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Abstract. We consider an ideal Fermi gas confined to a geometric structure consisting of a central region – the sample – connected to several infinitely extended ends – the reservoirs. Under physically reasonable assumptions on the propagation properties of the one-particle dynamics within these reservoirs, we show that the state of the Fermi gas relaxes to a steady state. We compute the expected value of various current observables in this steady state and express the result in terms of scattering data, thus obtaining a geometric version of the celebrated Landauer-Büttiker formula.

1 Introduction

The study of transport phenomena in the quantum regime has attracted a lot of interest over the last decades, especially within the realm of condensed matter physics. The main efforts have been devoted to the development of computational tools for the calculation of steady state properties of a confined quantum system (the sample) driven out of thermal equilibrium by mechanical or thermodynamical forces. This physical setup is conveniently described by an open-system model where the sample $\mathscr{S}$ is coupled to large (eventually infinitely extended) heat and particle reservoirs $\mathscr{R}_1, \mathscr{R}_2, \ldots$ (see Figure 1). Thermodynamical forces are implemented by the initial state of the joint system $\mathscr{S} + \mathscr{R}_1 + \mathscr{R}_2 + \cdots$. More precisely, each reservoir $\mathscr{R}_k$ is prepared in a thermal equilibrium state with its own intensive thermodynamic parameters: inverse temperature β_k, chemical potential $\mu_k, \ldots$ In the physics literature, this is sometimes called "the partitioned scenario", reflecting the fact that each reservoir has to be prepared individually before being connected to the sample. Mechanical forcing is obtained by imposing (possibly time dependent) potential bias in the reservoirs, the initial state of the system being a joint thermal equilibrium state of the coupled system $\mathscr{S} + \mathscr{R}_1 + \mathscr{R}_2 + \cdots$. This is the so called "partition free scenario", see [CCNS, C].

Whether such an open system, prepared in a given initial state, actually relaxes to a steady state is a more delicate question which can not be treated by formal arguments and requires a precise control of quantum dynamics. To the best of our knowledge, the first rigorous results on this fundamental problem of nonequilibrium quantum statistical mechanics were obtained by Lebowitz and Spohn [Sp1, Sp2, Sp3, LS] in the case of thermodynamical forcing. Besides providing simple and efficient criteria ensuring relaxation to a steady state in the van Hove scaling limit (weak coupling), they have also studied the basic thermodynamic properties of these steady states: strict positivity of entropy production and linear response

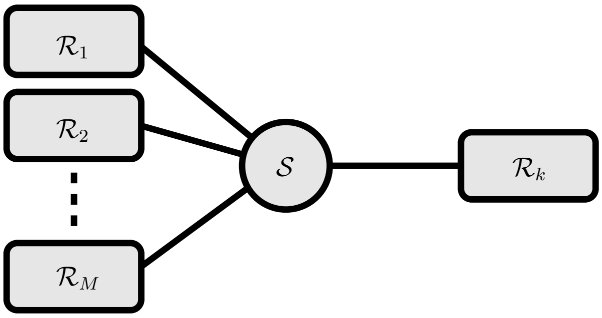

Figure 1: A sample $\mathscr{S}$ coupled to M reservoirs $\mathscr{R}_1, \ldots, \mathscr{R}_M$.

theory. In the same limit, Davies and Spohn have studied the linear response of confined quantum systems to mechanical drives [DSp]. These works rely on Davies' results on the weak coupling limit [D1, D2] (see also the recent extension of Davies' theory by Dereziński and de Roeck [DdR1, DdR2]) and therefore only provide a coarse time resolution of transport phenomena.

In these notes we shall consider the simplest case, beyond the weak coupling limit, amenable to rigorous analysis: the transport properties of an ideal Fermi gas (e.g., of an electronic gas in the approximation of independent electrons commonly used in solid state physics). Due to the absence of interactions, the nonequilibrium properties of such a gas can be derived from the quantum dynamics of a one-particle system. We shall concentrate more specifically on the Landauer-Büttiker formalism which relates the steady currents through a sample connected to several fermionic reservoirs at different chemical potentials to the scattering data associated with the coupling of the sample to the reservoirs (we shall provide a more detailed discussion of the Landauer-Büttiker formalism in Section 3.4.7).

Relaxation to a nonequilibrium steady state (NESS) for an ideal Fermi gas in the partitioned scenario was first obtained by Araki and Ho [AH]. These Authors studied the large time asymptotics of the isotropic XY spin chain prepared in a state with different temperatures on its left and and right ends (the XY chain can be mapped to an ideal Fermi gas on a 1D lattice by a Jordan-Wigner transformation). Their result has been extended to the anisotropic XY chain in [AP] using a different approach, advocated by Ruelle [R4], and based on scattering theory. In Ruelle's approach, the NESS is expressed in terms of the initial state of the gas and the Møller operator describing the scattering of a particle from the reservoirs by the sample (see Section 5.5). However, to derive the Landauer-Büttiker formula which expresses the steady state currents in terms of transmission probabilities (i.e., scattering matrix) requires further work. This was first achieved in [AJPP2, N] within the stationary formalism of scattering theory and for more general classes of ideal Fermi gases driven by thermodynamical forces (see also Section 7 in [AJPP1] and [CNWZ]).

In the case of mechanical forcing (in the partition-free scenario), a linearized Landauer-Büttiker formula (i.e., a formula for the conductivity of the sample) was obtained by Cornean *et al.* in [CJM, CDNP]. However, relaxation to a NESS did not follow from the linear response approach used in these works and was first proved in [CDP][1]. Finally, a complete (non-linear) Landauer-Büttiker formula for the steady currents was derived in [CGZ]. A unified treatment of the partitioned/partition-free NESS can be found in [CMP2].

In both scenarios a necessary condition for the coupled/biased system $\mathscr{S}+\mathscr{R}_1+\cdots$ to relax to a NESS is that its final, fully coupled/biased, one-particle Hamiltonian has empty singular spectrum. In that case, the NESS only depends on the initial states of the reservoirs and on the final one-particle Hamiltonian. It is, in particular, independent of the initial state of the sample and of the (possibly time-dependent) switching of the coupling/bias [CNZ, CMP2]. In fact, the presence of eigenvalues in the one-particle Hamiltonian of the fully coupled/biased system produces oscillations which prevent relaxation to a steady state [Ste, KKSG]. These oscillations are carried by the eigenfunctions of the Hamiltonian and hence are typically localized near the sample. Current measurements performed deep into the reservoirs are therefore immune to this effect [CGZ]. If the singular continuous spectrum of the final Hamiltonian is empty, then the oscillations induced by its eigenvalues can also be washed out by time-averaging the state of the system. The time-averaged state relax to a steady state which, however, depends on the initial state of the sample and on the history of the coupling/bias [AJPP2, CGZ, CJN].

Before turning to a detailed review of the content of these notes, let us mention some important results in the same line of research but which will not be covered here.

Ruelle's scattering approach also works in the presence of weak local interactions (i.e., many body interactions that are sufficiently well localized in position and momentum). In this case, the Møller operator of Hilbert space scattering theory is replaced by a Møller morphism acting on the C^*-algebra $\mathscr{O}$ of observables of the coupled system ($\mathscr{O}$ is typically the gauge invariant part of the C^*-algebra generated by fermionic creation/annihilation operators satisfying the canonical anti-commutation relations, see Section 3.2). This morphism can be constructed by controlling the Dyson expansion of the interaction picture propagator acting on $\mathscr{O}$, using the techniques of [BM1, BM2]. Relaxation to a NESS of a locally interacting Fermi gas in the partitioned scenario was first proved by Fröhlich *et al.* [DFG, FMU]. Linear response theory (including a central limit theorem) for such NESS was developed in [JOP1, JOP2, JPP]. Using similar techniques, a mathematical theory of basic thermodynamic processes in ideal and locally interacting Fermi gases has been developed in [FMSU]. A unified approach to both partitioned/partition-free NESS of locally interacting Fermi gases was developed in [CMP1, CMP2] where basic properties of the NESS Green-Keldysh correlation functions were also derived.

The spectral analysis of Liouvilleans provides an alternative to Ruelle's scattering approach to the construction of NESS. A Liouvillean for the coupled system $\mathscr{S}+\mathscr{R}_1+\cdots$ is an operator L acting on a Hilbert space which carries a representation of the C^*-algebra $\mathscr{O}$ and such that the group $t\mapsto \mathrm{e}^{\mathrm{i}tL}$ implements the dynamics (see [P2, DJP, JOPP]). For systems with finitely extended reservoirs the Liouvillean is essentially determined by the Hamiltonian. There is how-

[1]For identical intensive thermodynamic parameters, the partitioned/partition-free scenarios lead to distinct NESS.

ever much more freedom in the choice of a Liouvillean if the reservoirs are infinitely extended. The Liouvillean approach has been successfully used to prove return to equilibrium of a confined system connected to a single heat bath [JP1, JP2, JP3, JP4, Me, BFS3, DJ1, DJ2, FM]. An extension of this technique to nonequilibrium situations was developed in [JP6] to prove relaxation to a steady state of a N-level system coupled to several fermionic reservoirs. Merkli, Mück and Sigal have extended this result to the technically more involved case of bosonic reservoirs [MMS]. In these works, the steady state is characterized by a spectral resonance of a Liouvillean which is constructed with the help of operator algebraic techniques derived from the fundamental results of [HHW, To, Ta]. Due to the use of spectral deformation techniques in the resonance analysis, the method requires quite strong regularity assumptions on the coupling of the sample to the reservoir. It does however provide a very detailed information on the dependence of the NESS on this coupling (a convergent perturbative expansion). A similar approach was used by Fröhlich, Merkli and Sigal [FMS] to study the ionization process in a thermal field. We shall also mention a series of works by Abou Salem and Fröhlich [AF1, AF2, AF3] who exploit the Liouvillean approach to derive some of the basic laws of thermodynamics from microscopic quantum dynamics. We refer the reader to the article of Schach Møller [SM] in this volume for a detailed exposition of the spectral theory of some important classes of Liouvilleans.

A third approach to the relaxation problem has been developed by de Roeck and Kupiainen in [dRK1, dRK2] (see also [dR1]). It uses Davies' weak coupling approximation of the dynamics as a starting point for a systematic expansion of the true, fully coupled dynamics. The control of this expansion is technically more involved than the analysis required in the Liouvillean approach, but it is very robust and only requires minimal assumptions on the coupling to the reservoir (essentially the existence of the Davies approximation with a spectral gap). However, the method does not provide much information on the dependence of the NESS on the coupling.

The material presented in these notes is partly based on the PhD thesis of the first Author [Sa]. It can be read as a pedagogical introduction to some contemporary aspects of the mathematics of nonequilibrium quantum statistical mechanics. The main objectives are:

- To prove relaxation of an ideal Fermi gas under thermodynamical drive using Ruelle's approach and geometric time-dependent scattering theory based on the Mourre estimate. This framework has many advantages over the stationary scattering theory used in the previous works on the subject. Our main assumptions, which ensure good propagation properties at large distance from the sample, concerns the reservoirs. They are easily checked for reservoirs with a simple geometry. Mourre theory gives us a simultaneous control over the propagation properties and the singular spectrum of the coupled system. Finally, with the use of the two Hilbert space formalism, we avoid the decoupling of the sample by artificial boundary conditions. The scattering matrix obtained in this way is explicitly independent of any decoupling scheme, which represents a serious conceptual advantage.

- To show that the properly defined NESS expectation of a current observable can be expressed in terms of scattering data by a geometric version of the Landauer-Büttiker formula. Our approach has been deeply inspired by the works of Avron *et al.* [AEGS1, AEGS2, AEGS3] and more specifically [AEGSS] who treat the similar problem of charge transport in quantum pumps in the adiabatic regime (and prove the Büttiker-Prêtre-Thomas formula [BTP]).

Our main results are Proposition 5.14 and Theorem 5.15, which guarantee the existence and uniqueness of the NESS under physically reasonable conditions. Under a few additional assumptions, we prove a geometric version of the Landauer-Büttiker formula in Theorem 6.7.

The organization of these notes is as follows:

- In Section 2 we describe the necessary mathematical background for our work. The goal here is essentially to introduce the basic tools and the notation that will be used in the following sections.

- Section 3 is a brief introduction to nonequilibrium statistical mechanics of open quantum systems, and more specifically, -free fermionic systems. We introduce the concept of NESS and describe Ruelle's scattering method for its construction.

- Section 4 is a thorough discussion of commutators of Hilbert space operators and their use in spectral analysis. It introduces the elements of Mourre theory which will be necessary for controlling the singular spectrum and the propagation properties of quasi-free fermionic systems.

- Section 5 is dedicated to the construction of NESS using the geometric theory of multichannel scattering and propagation estimates.

- In Section 6 we discuss current observables and compute their expectation values in the NESS, deriving the geometric Landauer-Büttiker formula.

- The appendices A and B contain a few technical proofs that we deemed appropriate to be separated from the main part of these notes.

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2 Mathematical background

In this section we briefly review the necessary mathematical background. The main purpose is to setup our notation. The covered material is very basic and the exposition is in telegraphic style, without formal proofs. The readers familiar with spectral analysis in Hilbert spaces and operator algebras can safely jump over to the next section.

In Subsection 2.1 we introduce the fundamentals of spectral analysis of operators on a Hilbert space, paying particular attention to self-adjoint operators and to the scattering theory of the associated unitary groups. These are the common tools used in the mathematical study of quantum dynamics, i.e., solutions to the Schrödinger equation, either time-dependent or time-independent. Among the numerous techniques developed to study the properties of the solutions to this equation, those based on the work of Mourre will play a central role in these notes. These techniques will be the object of a more detailed discussion in Section 4.

Subsection 2.2 is a brief introduction to the theory of operator algebras and more particularly C^*-algebras. From the perspective of the material covered in these notes, the relevance of this subject is marginal. It does however play an important role in the more general context of the mathematical theory of quantum statistical mechanics. As we have already noted in the general introduction, the development of this theory saw a revival in the last decade, essentially revolving around transport problems in nonequilibrium systems. These recent developments were built upon the foundations of the algebraic approach to equilibrium quantum statistical mechanics developed in the 1960s and 1970s.

2.1 Spectral analysis and scattering theory

In this section we recall some fundamental results of spectral analysis of self-adjoint operators on a Hilbert space, as well as the basics of scattering theory. The material covered in this section is treated in full detail in [RS1]–[RS4].

2.1.1 Closed operators and bounded operators

If A, B are non-empty sets we denote by $\langle a, b\rangle$ the elements of the Cartesian product $A\times B$ so as to not generate confusion with the following notation.

Let $\mathcal{H}$ be a Hilbert space. We denote by

$$\begin{array}{ccc} \mathcal{H}\times\mathcal{H} & \longrightarrow & \mathbb{C} \\ \langle u, v\rangle & \mapsto & (u, v), \end{array}$$

the inner product of $\mathcal{H}$, which is anti-linear in its first argument and linear in its second one. Riesz' representation theorem guarantees that any continuous linear functional $\ell:\mathcal{H}\to\mathbb{C}$ can be written in the form $\ell(v) = (u, v)$ for some $u\in\mathcal{H}$. The ortho-complement of a subset $V\subset\mathcal{H}$ is defined by $V^\perp = \{u\in\mathcal{H}\,|\,(v,u) = 0 \text{ for all } v\in V\}$. It is a closed subspace of $\mathcal{H}$ and $V^{\perp\perp}$ is the smallest closed subspace of $\mathcal{H}$ containing V. An automorphism of $\mathcal{H}$ is a linear and isometric bijection from $\mathscr{H}$ onto itself. $\mathscr{H}\times\mathscr{H}$ equipped with its natural vector space structure and the inner product $(\langle u,v\rangle,\langle u',v'\rangle)=(u,u')+(v,v')$ is a Hilbert space and $\mathbb{K}:\langle x,y\rangle\mapsto\langle y,x\rangle$ and $\mathbb{J}:\langle x,y\rangle\mapsto\langle -y,x\rangle$ define automorphisms of $\mathscr{H}\times\mathscr{H}$. A net u_α in $\mathscr{H}$ converges weakly to $u\in\mathscr{H}$ if the net (v,u_α) converges to (v,u) for all $v\in\mathscr{H}$. In this case we write

$$\mathrm{w}-\lim_{\alpha} u_\alpha = u.$$

An operator on $\mathscr{H}$ is a linear map $A:\mathscr{D}\to\mathscr{H}$, where $\mathscr{D}$ is a subspace of $\mathscr{H}$. We say that $\mathscr{D}$ is the domain of A which we denote by $\mathrm{Dom}(A)$. A is densely defined if its domain is dense in $\mathscr{H}$. The range and the kernel of A are the subspaces $\mathrm{Ran}\,(A)\equiv\{Au\,|\,u\in\mathrm{Dom}(A)\}$ and $\mathrm{Ker}\,(A)\equiv\{u\in\mathrm{Dom}(A)\,|\,Au=0\}$ respectively. A is surjective if $\mathrm{Ran}\,(A)=\mathscr{H}$ and injective if $\mathrm{Ker}\,(A)=\{0\}$.

The graph of an operator A on $\mathscr{H}$ is the the subspace

$$\mathrm{Gr}\,(A)\equiv\{\langle u,Au\rangle\,|\,u\in\mathrm{Dom}(A)\},$$

of $\mathscr{H}\times\mathscr{H}$. The graph norm of A is the norm defined by $\|u\|_A=\|u\|+\|Au\|$ on $\mathrm{Dom}(A)$. An operator A is completely characterized by its graph. Moreover, a subspace $\mathscr{G}\subset\mathscr{H}\times\mathscr{H}$ is the graph of an operator iff $\langle 0,v\rangle\in\mathscr{G}$ implies $v=0$. If A and B are two operators such that $\mathrm{Gr}\,(A)\subset\mathrm{Gr}\,(B)$ we say that B is an extension of A and we write $A\subset B$. An operator A is closed if its graph is closed in $\mathscr{H}\times\mathscr{H}$, and this is the case iff $\mathrm{Dom}(A)$, equipped with the graph norm of A, is a Banach space. If A is both closed and bijective, then $\mathrm{Gr}\,(A^{-1})=\mathbb{K}\mathrm{Gr}\,(A)$ and thus A^{-1} is also closed. If the closure $\mathrm{Gr}\,(A)^{\mathrm{cl}}$ of the graph of A in $\mathscr{H}\times\mathscr{H}$ is a graph we say that A is closable and we define its closure as the operator A^{cl} such that $\mathrm{Gr}\,(A^{\mathrm{cl}})=\mathrm{Gr}\,(A)^{\mathrm{cl}}$. It is clear that A^{cl} is the smallest closed extension of A, that is to say that if B is closed and $A\subset B$, then $A^{\mathrm{cl}}\subset B$. An operator A is densely defined iff $\mathbb{J}(\mathrm{Gr}\,(A)^{\perp})$ is a graph. In this case, the adjoint of A is the operator A^* defined by $\mathrm{Gr}\,(A^*)=\mathbb{J}(\mathrm{Gr}\,(A)^{\perp})$. A^* is closed and its domain is given by

$$\mathrm{Dom}(A^*)=\{u\in\mathscr{H}\,|\sup_{v\in\mathrm{Dom}(A),\|v\|=1}|(u,Av)|<\infty\}.$$

$(A^*u,v)=(u,Av)$ holds for all $\langle u,v\rangle\in\mathrm{Dom}(A^*)\times\mathrm{Dom}(A)$, in particular $\mathrm{Ker}\,(A^*)=\mathrm{Ran}\,(A)^{\perp}$. A is closable iff A^* is densely defined. In this case $A^{\mathrm{cl}}=A^{**}$ and $A^{\mathrm{cl}\,*}=A^*$.

An operator A is bounded if there exists a constant C such that $\mathrm{Gr}\,(A)\subset\{\langle u,v\rangle\,|\,\|v\|\le C\|u\|\}$. One easily verifies that A is continuous as a map from $\mathrm{Dom}(A)$ to $\mathscr{H}$ iff it is bounded. A bounded operator is obviously closable and its closure coincide with its unique continuous extension to the closure of $\mathrm{Dom}(A)$. In particular a bounded densely defined operator A has a unique continuous extension A^{cl} with domain $\mathrm{Dom}(A^{\mathrm{cl}})=\mathscr{H}$. A^{cl} is closed and bounded. The collection of all bounded operators with domain $\mathscr{H}$ is denoted by $\mathscr{B}(\mathscr{H})$. It is a Banach algebra (actually a C^*-algebra, see Section 2.2) with norm

$$\|A\|\equiv\sup_{u\in\mathscr{H},\|u\|=1}\|Au\|. \tag{1}$$

By the closed graph theorem, an operator A with domain $\mathscr{H}$ is bounded iff it is closed. If A is bounded and densely defined, then $\mathrm{Dom}(A^*)=\mathscr{H}$ and A^* is bounded. Furthermore, $\|A^*\|=\|A\|$ and $\|A^*A\|=\|A\|^2$.

A bounded net A_α in $\mathscr{B}(\mathscr{H})$ is strongly (resp. weakly) convergent if the net $A_\alpha u$ is convergent (resp. weakly convergent) for every $u \in \mathscr{H}$. In this case, there exists $A \in \mathscr{B}(\mathscr{H})$ such that $\lim_\alpha A_\alpha u = Au$ for all $u \in \mathscr{H}$ (resp. $\lim_\alpha (u, A_\alpha v) = (u, Av)$ for all $u, v \in \mathscr{H}$), and we write $\mathrm{s}-\lim_\alpha A_\alpha = A$ (resp. $\mathrm{w}-\lim_\alpha A_\alpha = A$). If $A_\alpha^{(1)}, \ldots, A_\alpha^{(n)}$ are bounded nets in $\mathscr{B}(\mathscr{H})$ and $\mathrm{s}-\lim_\alpha A_\alpha^{(j)} = A^{(j)}$ for all j then $\mathrm{s}-\lim_\alpha A_\alpha^{(1)} \cdots A_\alpha^{(n)} = A^{(1)} \cdots A^{(n)}$.

The resolvent set of a closed operator A is defined by

$$\mathrm{Res}(A) = \{z \in \mathbb{C} \,|\, \mathrm{Ker}\,(A - z) = \{0\} \text{ and } \mathrm{Ran}\,(A - z) = \mathscr{H}\},$$

thus $z \in \mathrm{Res}(A)$ if and only if $(A - z) : \mathrm{Dom}(A) \to \mathscr{H}$ is a bijection. In this case, the operator $R_A(z) \equiv (A - z)^{-1} : \mathscr{H} \to \mathrm{Dom}(A)$ is called the resolvent of A at z. It is a closed operator with domain $\mathscr{H}$, and is thus bounded. It satisfies the functional equation $R_A(z) - R_A(z') = (z - z')R_A(z)R_A(z')$ (so called first resolvent equation) for all $z, z' \in \mathrm{Res}(A)$. If follows that for $z_0 \in \mathrm{Res}(A)$

$$R_A(z) = \sum_{n=0}^{\infty} R_A(z_0)^{n+1}(z - z_0)^n,$$

this Neumann series being norm convergent for $|z - z_0| < \|R_A(z_0)\|^{-1}$. Thus, the resolvent set of A is open, and the mapping $z \mapsto R_A(z)$ is an analytic function from $\mathrm{Res}(A)$ to $\mathscr{B}(\mathscr{H})$. The closed set $\mathrm{Sp}(A) \equiv \mathbb{C} \setminus \mathrm{Res}(A)$ is called the spectrum of A. A point $a \in \mathrm{Sp}(A)$ is an eigenvalue of A if there exists a non-zero vector $u \in \mathrm{Dom}(A)$ such that $Au = au$. We say that u is an eigenvector of A associated to the eigenvalue a.

If $\mathscr{H}$ and $\mathscr{K}$ are two Hilbert spaces, most of the preceding facts easily generalize to linear maps A from $\mathrm{Dom}(A) \subset \mathscr{H}$ to $\mathscr{K}$. We denote by $\mathscr{B}(\mathscr{H}, \mathscr{K})$ the Banach space of continuous operators from $\mathscr{H}$ to $\mathscr{K}$ equipped with the norm (1).

2.1.2 Self-adjoint operators

An operator A is called symmetric if $A \subset A^*$, self-adjoint if $A = A^*$, and essentially self-adjoint if $A^{**} = A^*$. An essentially self-adjoint operator A is closable and its closure $A^{\mathrm{cl}} = A^{**}$ is self-adjoint. In this case, we say that $\mathrm{Dom}(A)$ is a core of A^{cl}.

An operator A is symmetric if and only if $(u, Au) \in \mathbb{R}$ for all $u \in \mathrm{Dom}(A)$. Such an operator is self-adjoint iff $\mathrm{Ran}\,(A \pm \mathrm{i}) = \mathscr{H}$ and it is essentially self-adjoint iff $\mathrm{Ran}\,(A \pm \mathrm{i})$ is dense in $\mathscr{H}$.

If $\mathscr{K}$ is a closed subspace of $\mathscr{H}$ then $\mathscr{H} = \mathscr{K} \oplus \mathscr{K}^\perp$, i.e., any $u \in \mathscr{H}$ has a unique representation $u = x + y$ with $x \in \mathscr{K}$ and $y \in \mathscr{K}^\perp$. Moreover the Pythagoras theorem $\|u\|^2 = \|x\|^2 + \|y\|^2$ holds. The decomposition $u = x + y$ defines a bounded operator $P : u \mapsto x$ satisfying $P = P^2 = P^*$. We call P the orthogonal projection onto $\mathscr{K}$. Note that $Q = I - P$ is the orthogonal projection onto $\mathscr{K}^\perp$. Reciprocally, if $P \in \mathscr{B}(\mathscr{H})$ satisfies $P = P^2 = P^*$ then it is the orthogonal projection onto the closed subspace $\mathrm{Ran}\,(P) = \mathrm{Ker}\,(I - P)$ and $I - P$ is the orthogonal projection onto $\mathrm{Ker}\,(P) = \mathrm{Ran}\,(I - P)$.

If $\mathscr{K}$ is a closed subspace of $\mathscr{H}$ and J is an operator with domain $\mathscr{H}$ such that $\|Ju\| = \|u\|$ for all $u \in \mathscr{K}$ and $Ju = 0$ for all $u \in \mathscr{K}^\perp$ then $\mathrm{Ker}\,(J) = \mathscr{K}^\perp$ and $\mathscr{R} \equiv \mathrm{Ran}\,(J)$ is a closed subspace of $\mathscr{H}$. J is thus a isometric bijection from $\mathscr{K}$ into $\mathscr{R}$. We say that J is a partial isometry with initial space $\mathscr{K}$ and final space $\mathscr{R}$. One verifies that JJ^* is the orthogonal projection onto $\mathscr{R}$ and J^*J is the orthogonal projection onto $\mathscr{K}$. If $\mathscr{K} = \mathscr{R} = \mathscr{H}$ then $JJ^* = J^*J = I$ and J is unitary.

If A is self-adjoint, then $\mathrm{Sp}(A) \subset \mathbb{R}$. If we also have that $\mathrm{Sp}(A) \subset [0,\infty[$, then A is called positive and we write $A \geq 0$. A self-adjoint operator is positive if and only if $(u, Au) \geq 0$ for all $u \in \mathrm{Dom}(A)$. If C is a closed operator then C^*C with the domain $\mathrm{Dom}(C^*C) = \{u \in \mathrm{Dom}(C) \,|\, Cu \in \mathrm{Dom}(C^*)\}$ is positive. Conversely, every positive operator is of this form.

Every closed operator A has a unique polar decomposition $A = J|A|$ where $|A| \geq 0$ and J is a partial isometry with initial space $\mathrm{Ran}\,(A^*)^{\mathrm{cl}} = \mathrm{Ker}\,(A)^{\perp}$ and final space $\mathrm{Ran}\,(A)^{\mathrm{cl}} = \mathrm{Ker}\,(A^*)^{\perp}$. Moreover, $|A|$ is the square root of the positive operator A^*A constructed with the help of functional calculus which we shall now describe.

Spectral theorem 1. Let $B_b(\mathbb{R})$ be the algebra of bounded Borel functions from $\mathbb{R}$ to $\mathbb{C}$. If A is self-adjoint, there exists a unique morphism $\phi_A : B_b(\mathbb{R}) \to \mathscr{B}(\mathscr{H})$ such that

(i) $\phi_A(\overline{f}) = \phi_A(f)^*$.

(ii) $\|\phi_A(f)\| \leq \sup_{a\in\mathrm{Sp}(A)} |f(a)|$.

(iii) If $\lim_n f_n(a) = f(a)$ for all $a \in \mathrm{Sp}(A)$ and $\sup_{n,a\in\mathrm{Sp}(a)} |f_n(a)| < \infty$ then

$$\lim_n \phi_A(f_n)u = \phi_A(f)u,$$

for all $u \in \mathscr{H}$.

(iv) If $f \geq 0$ then $\phi_A(f) \geq 0$.

(v) If $Au = au$ then $\phi_A(f)u = f(a)u$.

(vi) If $z \in \mathrm{Res}(A)$ and $f(a) = (a-z)^{-1}$ then $\phi_A(f) = R_A(z)$.

We call this morphism the functional calculus associated with A and we write $f(A) = \phi_A(f)$. We say that a bounded operator B commutes with A if $Bf(A) = f(A)B$ for all $f \in B_b(\mathbb{R})$. A subspace $\mathscr{K} \subset \mathscr{H}$ is A-invariant if $f(A)\mathscr{K} \subset \mathscr{K}$ for all $f \in B_b(\mathbb{R})$. It reduces A if in addition $\mathscr{K}^{\perp}$ is also A-invariant. If $\mathscr{K}$ reduces A we define the part of A in $\mathscr{K}$ to be the self-adjoint operator on $\mathrm{Dom}(A) \cap \mathscr{K}$ obtained by restricting A to this subspace. We also define the part of the spectrum of A in $\mathscr{K}$ as $\mathrm{Sp}(A|\mathscr{K}) \equiv \mathrm{Sp}(A|_{\mathscr{K}\cap\mathrm{Dom}(A)})$.

Spectral theorem 2. It follows from the functional calculus that for all $u \in \mathscr{H}$ the map $f \mapsto (u, f(A)u)$ is a continuous linear functional on $C_\infty(\mathbb{R})$, the Banach space of continuous functions from $\mathbb{R}$ to $\mathbb{C}$ which tend to 0 at infinity, equipped with the norm $\|f\|_\infty \equiv \sup_{x\in\mathbb{R}} |f(x)|$. The Riesz-Markov theorem implies that there exists a finite measure μ_u, with $\mu_u(\mathbb{R}) = \|u\|^2$, and such that

$$(u, f(A)u) = \int f(a)\,\mathrm{d}\mu_u(a).$$

μ_u is the spectral measure of A associated with u.

Let $u \in \mathscr{H}$ and $\mathscr{H}_u = \{f(A)u \,|\, f \in C_\infty(\mathbb{R})\}^{\mathrm{cl}}$. The map $f \mapsto f(A)u$ from $C_\infty(\mathbb{R}) \to \mathscr{H}_u$ satisfies $\|f(A)u\| = \|f\|_{L^2(\mathbb{R},\mathrm{d}\mu_u)}$. It extends continuously to a unitary operator $U_u : L^2(\mathbb{R}, \mathrm{d}\mu_u) \to \mathscr{H}_u$ such that, if M_g denotes the multiplication operator $f \mapsto gf$ on $L^2(\mathbb{R}, \mathrm{d}\mu_u)$, $U_u M_g = g(A)U_u$. If $\mathscr{H}$ is separable, one can easily show that there exists a countable family $(u_n)_{n\in N} \subset \mathscr{H}$ such that $\mathscr{H} = \oplus_{n\in N}\mathscr{H}_{u_n}$. In this way we obtain a unitary map $U : \oplus_{n\in N} L^2(\mathbb{R}, \mathrm{d}\mu_n) \to \mathscr{H}$ such that, if g denotes the operator $\oplus_n u_n \mapsto \oplus_n g u_n$, then $Ug = g(A)U$. Alternatively stated, A is unitarily equivalent to the operator of multiplication by the variable a in the space $\oplus_{n\in N} L^2(\mathbb{R}, \mathrm{d}\mu_n(a))$.

One can show that $\mathscr{H} = \mathscr{H}_{\mathrm{pp}}(A) \oplus \mathscr{H}_{\mathrm{ac}}(A) \oplus \mathscr{H}_{\mathrm{sc}}(A)$ where

$$\begin{aligned}
\mathscr{H}_{\mathrm{pp}}(A) &\equiv \{u \in \mathscr{H} \,|\, \mu_u \text{ is purely atomic}\} \cup \{0\},\\
\mathscr{H}_{\mathrm{ac}}(A) &\equiv \{u \in \mathscr{H} \,|\, \mu_u \text{ is Lebesgue-absolutely continuous}\} \cup \{0\},\\
\mathscr{H}_{\mathrm{sc}}(A) &\equiv \{u \in \mathscr{H} \,|\, \mu_u \text{ is Lebesgue-singular without atoms}\} \cup \{0\},
\end{aligned}$$

are mutually orthogonal subspaces reducing A. We denote by $P_{\mathrm{pp}}(A)$, $P_{\mathrm{ac}}(A)$ and $P_{\mathrm{sc}}(A)$ the orthogonal projections onto these subspaces and we define A_{pp}, A_{ac}, and A_{sc} to be the parts of A in each of these subspaces. $\mathscr{H}_{\mathrm{pp}}(A)$ is the subspace spanned by the eigenvectors of A. The pure point, absolutely continuous, and singular spectra of A are defined by

$$\begin{aligned}
\mathrm{Sp}_{\mathrm{pp}}(A) &\equiv \{a \in \mathbb{R} \,|\, a \text{ is an eigenvalue of } A\},\\
\mathrm{Sp}_{\mathrm{ac}}(A) &\equiv \mathrm{Sp}(A_{\mathrm{ac}}),\\
\mathrm{Sp}_{\mathrm{sc}}(A) &\equiv \mathrm{Sp}(A_{\mathrm{sc}}),
\end{aligned}$$

and we have that $\mathrm{Sp}(A) = \mathrm{Sp}_{\mathrm{pp}}(A)^{\mathrm{cl}} \cup \mathrm{Sp}_{\mathrm{ac}}(A) \cup \mathrm{Sp}_{\mathrm{sc}}(A)$.

The singular spectrum of A is $\mathrm{Sp}_{\mathrm{sing}}(A) = \mathrm{Sp}_{\mathrm{pp}}(A)^{\mathrm{cl}} \cup \mathrm{Sp}_{\mathrm{sc}}(A)$. Its discrete spectrum is the set $\mathrm{Sp}_{\mathrm{disc}}(A)$ of all its isolated eigenvalues a having finite multiplicity, i.e., such that the corresponding eigenspace $\mathrm{Ker}\,(A-a)$ is finite dimensional. The essential spectrum of A is $\mathrm{Sp}_{\mathrm{ess}}(A) = \mathrm{Sp}(A) \setminus \mathrm{Sp}_{\mathrm{disc}}(A)$.

Spectral theorem 3. If 1_Δ is the indicator function of a Borel set $\Delta \subset \mathbb{R}$, then $E_A(\Delta) \equiv 1_\Delta(A)$ is an orthogonal projection. It is the spectral projection of A associated with Δ. Its image reduces A and we have that $\mathrm{Sp}(A|\mathrm{Ran}\,E_\Delta(A)) = \mathrm{Sp}(A) \cap \Delta \subset \Delta$ and $\mathrm{Sp}(A|\mathrm{Ker}\,E_\Delta(A)) \cap \Delta$ is empty. The family $\{E_\Delta(A) \,|\, \Delta \subset \mathbb{R} \text{ measurable}\}$ is called the spectral family of A. Stone's formula relates the spectral family to the resolvent of A: for all $u \in \mathscr{H}$ one has

$$\frac{1}{2}(E_A([a,b]) + E_A(]a,b[))u = \lim_{\varepsilon\downarrow 0} \frac{1}{2\pi\mathrm{i}} \int_a^b (R_A(a+\mathrm{i}\varepsilon)u - R_A(a-\mathrm{i}\varepsilon)u)\,\mathrm{d}a, \tag{2}$$

and, in particular, if a, b are not eigenvalues of A,

$$E_A([a,b])u = E_A(]a,b[)u = \lim_{\varepsilon\downarrow 0} \frac{1}{2\pi\mathrm{i}} \int_a^b (R_A(a+\mathrm{i}\varepsilon)u - R_A(a-\mathrm{i}\varepsilon)u)\,\mathrm{d}a.$$

Alternatively, the spectral family of A can be interpreted as a measure with values in the orthogonal projections of $\mathcal{H}$. It is thus related to the spectral measures previously introduced by writing $\mathrm{d}\mu_u(a) = (u, \mathrm{d}E_A(a)u)$ and we can formulate the functional calculus as

$$(u, f(A)v) = \int f(a)(u, \mathrm{d}E_A(a)v).$$

We also use the conventional notation $F(A \in \Delta) = E_\Delta(A)$ and, by extension, $F(A \geq a) = E_{[a,\infty[}(A)$, *etc...*

The following criterion for the absence of singular spectrum is often useful. Let Δ be a bounded open interval in $\mathbb{R}$ and assume that there exists a dense set $\mathcal{D} \subset \mathcal{H}$ such that

$$\sup_{\mathrm{Re}\,(z)\in\Delta, \mathrm{Im}\,(z)\neq 0} |(f, R_A(z)f)| < \infty,$$

for all $f \in \mathcal{D}$. It follows that $\mathrm{Sp}_{\mathrm{sing}}(A) \cap \Delta = \emptyset$, the spectrum of A in Δ is purely absolutely continuous.

Spectral theorem 4. For $n \in \overline{\mathbb{N}} \equiv \mathbb{N} \cup \{\infty\}$ we write

$$[1:n] \equiv \begin{cases} \emptyset & \text{if} \quad n = 0; \\ \{1, \ldots, n\} & if \quad n \in \mathbb{N}; \\ \mathbb{N}^* & if \quad n = \infty. \end{cases}$$

A function $n : \mathbb{R} \to \overline{\mathbb{N}}$ is measurable if $n^{-1}(\{k\})$ is measurable for all $k \in \overline{\mathbb{N}}$. A family of separable Hilbert spaces $(\mathfrak{h}_a)_{a\in\mathbb{R}}$ is measurable if $n(a) \equiv \dim \mathfrak{h}_a \in \overline{\mathbb{N}}$ defines a measurable function. Let μ be a σ-finite Borel measure on $\mathbb{R}$. Suppose that for μ-almost every $a \in \mathbb{R}$, $(e_n(a))_{n\in[1:n(a)]}$ is an orthonormal basis of $\mathfrak{h}_a$. By setting $e_n(a) = 0$ when $n > n(a)$ and when the basis $(e_n(a))_{n\in[1:n(a)]}$ is not defined, we can assume that $e_n(a)$ is defined for every $a \in \mathbb{R}$, $n \in \mathbb{N}$ (such a family is called a measurable orthonormal basis). Let X_0 be the set of functions $u : a \mapsto u(a)$ defined μ-almost everywhere on $\mathbb{R}$, with values in $\cup_{a\in\mathbb{R}}\mathfrak{h}_a$, such that $u(a) \in \mathfrak{h}_a$ for μ-almost all $a \in \mathbb{R}$ and $a \mapsto (e_n(a), u(a))_{\mathfrak{h}_a}$ are measurable for all $n \in \overline{\mathbb{N}}$. If $u, v \in X_0$ is it clear that $a \mapsto (u(a), v(a))_{\mathfrak{h}_a}$ is also measurable. Two functions $u, v \in X_0$ are equivalent if they agree μ-almost everywhere. The collection of equivalence classes of elements of X_0 such that $\|u\|^2 \equiv \int \|u(a)\|^2_{\mathfrak{h}_a} \mathrm{d}\mu(a) < \infty$ is a separable Hilbert space with the inner product $(u, v) = \int (u(a), v(a))_{\mathfrak{h}_a} \mathrm{d}\mu(a)$. This space is independent of choice of the family $(e_n(a))_{n\in[1:n(a)]}$, up to an isomorphism. We call it the direct integral of the family $(\mathfrak{h}_a)_{a\in\mathbb{R}}$ and we denote it by

$$\int^{\oplus} \mathfrak{h}_a \mathrm{d}\mu(a). \tag{3}$$

The spaces $\mathfrak{h}_a$ are called the fibers of this space. If one assumes that $\mathfrak{h}^k \equiv \ell^2([1:k])$, the Hilbert space of dimension k, and $\Delta_k \equiv \{a \,|\, \dim \mathfrak{h}_a = k\}$ for $k \in \overline{\mathbb{N}}$, one can show that the space (3) is isomorphic to the space

$$\bigoplus_{k\in\overline{\mathbb{N}}} L^2(\Delta_k, \mathrm{d}\mu) \otimes \mathfrak{h}^k.$$

If $t(a) \in \mathscr{B}(\mathfrak{h}_a)$ for μ-almost all $a \in \mathbb{R}$ with $C \equiv \mu - \operatorname{esssup}_{a\in\mathbb{R}} \|t(a)\| < \infty$ and if $(u(a), t(a)v(a))$ is measurable for all measurable functions u, v, we say that $t(\cdot)$ is a μ-measurable family of bounded operators. In this case, $(Tu)(a) \equiv t(a)u(a)$ defines a bounded operator T on the Hilbert space (3) and $\|T\| = C$. We refer to Chapter 7 of [BS] for more details.

If A is a self-adjoint operator on the separable Hilbert space $\mathscr{H}$, then there exists a measure μ, a measurable family of Hilbert spaces $(\mathfrak{h}_a)_{a\in\mathbb{R}}$ and a unitary map

$$U : \mathscr{H} \to \int^{\oplus} \mathfrak{h}_a \mathrm{d}\mu(a),$$

such that

$$\mathrm{Dom}(A) = \{u \in \mathscr{H} \mid \int a^2 \|(Uu)(a)\|^2_{\mathfrak{h}_a} \mathrm{d}\mu(a) < \infty\},$$

and, for all $u \in \mathrm{Dom}(A)$, $(UAu)(a) = a(Uu)(a)$ for μ-almost all $a \in \mathbb{R}$.

If the spectrum of A is pure point, then the measure μ is purely atomic. Its atoms are the eigenvalues a of A and the fibers $\mathfrak{h}_a$ are the corresponding eigenspaces of A. If the spectrum of A is purely absolutely continuous, one can choose μ to be the Lebesgue measure. In this case the set

$$\{u \in \mathscr{H} \mid \operatorname*{ess-sup}_{a\in\mathbb{R}} \|(Uu)(a)\|_{\mathfrak{h}_a} < \infty\},$$

is a dense subspace of $\mathscr{H}$. This applies in particular to the operators $A_{\mathrm{pp}} = A|_{\mathscr{H}_{\mathrm{pp}}(A)}$ and $A_{\mathrm{ac}} = A|_{\mathscr{H}_{\mathrm{ac}}(A)}$.

If $B \in \mathscr{B}(\mathscr{H})$ commutes with A, there exists a μ-measurable family $b(\cdot)$ of bounded operators such that $(UBf)(a) = b(a)(Uf)(a)$ for μ-almost all $a \in \mathbb{R}$.

The Helffer-Sjöstrand Formula. For sufficiently smooth functions f, it is possible to give an explicit representation of the operator $f(A)$. Multiple constructions of this type exist. We will mainly use the Helffer-Sjöstrand formula, which is well adapted to the case where $f \in S(\mathbb{R})$ where

$$S(\mathbb{R}) \equiv \{f \in C^\infty(\mathbb{R}) \mid \sup_{x\in\mathbb{R}} \langle x\rangle^{\beta+n} |\partial_x^n f(x)| < \infty \text{ for some } \beta > 0 \text{ and all } n \ge 0\},$$

(with $\langle x\rangle \equiv (1+x^2)^{1/2}$) and in particular for $f \in C_0^\infty(\mathbb{R})$, the set of infinitely differentiable functions which vanish outside of a compact set. We denote by $\operatorname{supp} f$ the support of such a function, that is to say the smallest closed set $F \subset \mathbb{R}$ such that $f = 0$ on $\mathbb{R} \setminus F$.

For $f \in C^\infty(\mathbb{R})$ and $n \in \mathbb{N}$, let $\tilde{f} : \mathbb{C} \to \mathbb{C}$ be defined by

$$\tilde{f}(x + \mathrm{i}y) \equiv \chi(y\langle x\rangle^{-1}) \sum_{j=0}^{n+1} f^{(j)}(x) \frac{(\mathrm{i}y)^j}{j!}, \tag{4}$$

where $\chi \in C_0^\infty(]-1,1[)$ is such that $\chi(y) = 1$ in a neighborhood of $y = 0$. We remark that, apart from the factor χ, (4) is a formal Taylor expansion of order n about the point x of the function $f(x+\mathrm{i}y)$. For functions of $z = x + \mathrm{i}y$ we will use the notation from complex analysis $\partial = (\partial_x - \mathrm{i}\partial_y)/2$, $\bar\partial = (\partial_x + \mathrm{i}\partial_y)/2$ and $\mathrm{d}z = \mathrm{d}x + \mathrm{i}\mathrm{d}y$, $\mathrm{d}\bar{z} = \mathrm{d}x - \mathrm{i}\mathrm{d}y$. A simple calculation yields

$$\bar\partial\partial^j \tilde{f}(x) = 0, \qquad \partial^j \tilde{f}(x) = f^{(j)}(x),$$

for all $x \in \mathbb{R}$ and $j \in \{0, \dots, n\}$, and this is why $\tilde{f}$ is called an almost-analytic extension of f of order n. One easily shows that:

(i) There exists a constant C (which depends only on n) such that

$$\int |(\bar{\partial}\tilde{f})(x + \mathrm{i}y)| \, |y|^{-1-j} \, \mathrm{d}y \le C \sum_{k=0}^{n+2} \langle x \rangle^{k-1-j} |f^{(k)}(x)|, \tag{5}$$

for $j \in \{0, \dots, n\}$.

(ii) If $f \in C_0^\infty(\mathbb{R})$ then $\tilde{f} \in C_0^\infty(\mathbb{C})$ and

$$\operatorname{supp} \tilde{f} \subset \{z = x + \mathrm{i}y \,|\, x \in \operatorname{supp} f, |y| \le \langle x \rangle\}.$$

Moreover, the functional calculus implies that $\|(x + \mathrm{i}y - A)^{-1}\| \le |y|^{-1}$. Using these properties and starting with Stone's formula (2) an integration by parts shows that

$$\frac{1}{j!} f^{(j)}(A) = -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial}\tilde{f}(x + \mathrm{i}y)(x + \mathrm{i}y - A)^{-1-j} \, \mathrm{d}x\mathrm{d}y = \frac{1}{2\pi\mathrm{i}} \int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)(z - A)^{-1-j} \mathrm{d}z \wedge \mathrm{d}\bar{z}, \tag{6}$$

for $j \in \{0, \dots, n\}$ and $f \in C_0^\infty(\mathbb{R})$ (see [HS] and [D4], Section 2.2 for a direct approach to spectral theory from the Helffer-Sjöstrand formula). An approximation argument further shows that (6) remains valid if $f \in C^{n+2}(\mathbb{R})$ is such that

$$\int \langle x \rangle^{k-1} |f^{(k)}(x)| \, \mathrm{d}x < \infty,$$

for $k \in \{0, \dots, n+2\}$ and in particular if $f \in S(\mathbb{R})$.

2.1.3 Compact operators

An operator $C \in \mathscr{B}(\mathscr{H})$ is compact if $\{Cu \,|\, u \in \mathscr{H}, \|u\| = 1\}^{\mathrm{cl}}$ is a compact subset of $\mathscr{H}$. The set $\mathscr{L}^\infty(\mathscr{H})$ of all compact operators on $\mathscr{H}$ is a closed two-sided $*$-ideal of the C^*-algebra $\mathscr{B}(\mathscr{H})$ (see Section 2.2).

Let A be a self-adjoint operator on $\mathscr{H}$. An operator B on the same Hilbert space is called A-bounded (resp. A-compact) if $\mathrm{Dom}(A) \subset \mathrm{Dom}(B)$ and there exists $z_0 \in \mathrm{Res}(A)$ such that $B(z_0 - A)^{-1}$ is bounded (resp. compact). In this case, it follows from the first resolvent identity that $B(z - A)^{-1}$ is bounded (resp. compact) for all $z \in \mathrm{Res}(A)$. Weyl's theorem asserts that if B is symmetric and A-compact then $A + B$ is self-adjoint on $\mathrm{Dom}(A)$ and $\mathrm{Sp}_{\mathrm{ess}}(A + B) = \mathrm{Sp}_{\mathrm{ess}}(A)$.

In the remaining of this subsection, we shall assume that $\mathscr{H}$ is separable. An operator on $\mathscr{H}$ is finite rank if $\mathrm{Ran}\,(A)$ is finite dimensional. The set $\mathscr{L}_{\mathrm{fin}}(\mathscr{H})$ of all finite rank operators on $\mathscr{H}$ is a $*$-subalgebra of $\mathscr{B}(\mathscr{H})$ and is dense in $\mathscr{L}^\infty(\mathscr{H})$ (in the norm topology of $\mathscr{B}(\mathscr{H})$). This leads to the result that if $C \in \mathscr{L}^\infty(\mathscr{H})$ and $\mathrm{w} - \lim_\alpha u_\alpha = u$ then $\lim_\alpha Cu_\alpha = Cu$.

If $A \in \mathscr{L}^\infty(\mathscr{H})$ is self-adjoint, then $\mathrm{Sp}_{\mathrm{cont}}(A) = \mathrm{Sp}_{\mathrm{ac}}(A) \cup \mathrm{Sp}_{\mathrm{sc}}(A)$ is empty. Furthermore, $\mathrm{Sp}_{\mathrm{pp}}(A)$ is at most countable and can only accumulate at 0. For all $a \in \mathrm{Sp}_{\mathrm{pp}}(A) \setminus \{0\}$, $\mathrm{Ker}\,(A - a)$ is finite dimensional. We can therefore deduce that there exists a set N, which is at most countable, such that $A = \sum_{n\in N} a_n u_n(u_n,\cdot)$ where $\{a_n \mid n \in N\} = \mathrm{Sp}_{\mathrm{pp}}(A) \setminus \{0\}$ and $(u_n)_{n\in N}$ is an orthonormal family of eigenvectors $Au_n = a_n u_n$. More generally, if $A \in \mathscr{L}^\infty(\mathscr{H})$, it follows from the polar decomposition $A = J|A|$ that

$$A = \sum_{n\in N(A)} \kappa_n(A)\, v_n(u_n,\cdot).$$

The numbers $\kappa_n(A) > 0$ are called singular values of A. Their squares $\kappa_n(A)^2$ are eigenvalues of the positive compact operator A^*A. The u_n form an orthonormal family of eigenvectors $A^*Au_n = \kappa_n(A)^2 u_n$ while the $v_n = Ju_n$ form an orthonormal family of eigenvectors of AA^*, $AA^* v_n = \kappa_n(A)^2 v_n$.

A simple but very convenient compactness criterion on the Hilbert space $L^2(\mathbb{R}^n)$ is due to Rellich. Let F and G be two measurable functions on $\mathbb{R}^n$ with the following property: for any $K > 0$ there exists $R > 0$ such that $|F(x)| > K$ and $|G(x)| > K$ for almost every $x \in \mathbb{R}^n$ with $|x| > R$. Denote by F and G the operators of multiplication by the corresponding functions on $L^2(\mathbb{R}^n)$ and let $\mathscr{F} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ denote the Fourier transform. If C is a bounded operator such that FC and $G\mathscr{F}C$ are bounded then C is compact.

For $1 \le p < \infty$, the von Neumann-Schatten class

$$\mathscr{L}^p(\mathscr{H}) \equiv \left\{ A \in \mathscr{L}^\infty(\mathscr{H}) \,\middle|\, \|A\|_p \equiv \left(\sum_{n\in N(A)} \kappa_n(A)^p \right)^{1/p} < \infty \right\},$$

is a two-sided $*$-ideal of $\mathscr{B}(\mathscr{H})$ and a Banach space equipped with the norm $\|\cdot\|_p$. For all $C \in \mathscr{L}^p(\mathscr{H})$ and $B \in \mathscr{B}(\mathscr{H})$, $\|BC\|_p \le \|B\|\,\|C\|_p$. We will mainly focus on the space $\mathscr{L}^1(\mathscr{H})$, the elements of which are called trace class operators on $\mathscr{H}$. For all $A \in \mathscr{L}^1(\mathscr{H})$ and for any orthonormal basis $(u_i)_{i\in I}$ of $\mathscr{H}$, the series $\sum_{i\in I}(u_i, Au_i)$ is absolutely convergent. Furthermore, its sum is independent of the choice of basis, and we call this sum the trace of A, denoting it by $\mathrm{tr}(A)$. One clearly has

$$\mathrm{tr}(A) = \sum_{a\in \mathrm{Sp}(A)} a \dim \mathrm{Ker}\,(A - a).$$

Moreover, the following inequality holds

$$|\mathrm{tr}(A)| \le \sum_{n\in N(a)} \kappa_n(A) = \mathrm{tr}(|A|) = \|A\|_1, \tag{7}$$

for all $A \in \mathscr{L}^1(\mathscr{H})$. More generally, $A \in \mathscr{L}^p(\mathscr{H})$ if and only if $|A|^p \in \mathscr{L}^1(\mathscr{H})$ and $\|A\|_p = \mathrm{tr}(|A|^p)^{1/p}$. If $\dim \mathscr{H} < \infty$ then $\mathscr{L}^p(\mathscr{H}) = \mathscr{B}(\mathscr{H})$ for all $1 \le p \le \infty$ and in this case it is a well known fact that the trace is cyclic, that is to say that $\mathrm{tr}(AB) = \mathrm{tr}(BA)$ for all $A, B \in \mathscr{B}(\mathscr{H})$. In the infinite dimensional case, the cyclic property of the trace holds when one of the operators involved is trace class: if $A \in \mathscr{L}^1(\mathscr{H})$ and $B \in \mathscr{B}(\mathscr{H})$ then

$$\mathrm{tr}(AB) = \mathrm{tr}(BA).$$

If $A \in \mathscr{L}^1(\mathscr{H})$, it follows from the estimate (7) that the infinite product

$$\det(I + A) = \prod_{a \in \mathrm{Sp}(A)} (1 + a)^{\dim \mathrm{Ker}(A-a)},$$

is convergent and satisfies

$$|\det(1 + A)| \le \mathrm{e}^{\|A\|_1}.$$

Let $1 \le p, q \le \infty$ be such that $p^{-1} + q^{-1} = 1$. If $A \in \mathscr{L}^p(\mathscr{H})$ and $B \in \mathscr{L}^q(\mathscr{H})$ then $AB \in \mathscr{L}^1(\mathscr{H})$ and the Hölder inequality $\|AB\|_1 \le \|A\|_p \|B\|_q$ holds. If $1 < p \le \infty$, the topological dual of $\mathscr{L}^p(\mathscr{H})$ is $\mathscr{L}^q(\mathscr{H})$. The dual of $\mathscr{L}^1(\mathscr{H})$ is $\mathscr{B}(\mathscr{H})$. The Banach space $\mathscr{L}^p(\mathscr{H})$ is thus reflexive if $1 < p < \infty$, but not if $p = 1$ or $p = \infty$. In all cases the duality is given by $\langle A, B\rangle \mapsto \mathrm{tr}(AB)$.

Finally, we note that if A_α is a bounded net in $\mathscr{B}(\mathscr{H})$ such that $\mathrm{s}-\lim\limits_{\alpha} A_\alpha = A \in \mathscr{B}(\mathscr{H})$ and $B \in \mathscr{L}^p(\mathscr{H})$ then $\lim_\alpha A_\alpha B = AB$ holds in $\mathscr{L}^p(\mathscr{H})$.

2.1.4 Unitary groups and scattering theory

If H is self-adjoint, the functional calculus shows that $U(t) \equiv \mathrm{e}^{\mathrm{i}tH}$, $t \in \mathbb{R}$, defines a family of operators on $\mathscr{H}$ such that

(i) $U(t)$ is unitary.

(ii) $U(0) = I$.

(iii) $U(t)U(s) = U(t + s)$.

(iv) For all $u \in \mathscr{H}$, $t \mapsto U(t)u$ is a continuous function from $\mathbb{R}$ to $\mathscr{H}$.

We call such a family $\{U(t) \,|\, t \in \mathbb{R}\}$ a strongly continuous unitary group. Stone's theorem states the converse; namely that if $\{U(t) \,|\, t \in \mathbb{R}\}$ is a strongly continuous unitary group on $\mathscr{H}$, then there exists a self-adjoint operator H such that $U(t) = \mathrm{e}^{\mathrm{i}tH}$. Furthermore,

$$Hu = \lim_{t \to 0} \frac{U(t)u - u}{\mathrm{i}t},$$

$\mathrm{Dom}(H)$ being the subspace of all $u \in \mathscr{H}$ such that the above limit exists.

Let H be a self-adjoint operator on $\mathscr{H}$. The "core theorem" states that if $\mathscr{D} \subset \mathrm{Dom}(H)$ is a dense subspace of $\mathscr{H}$ such that $\mathrm{e}^{\mathrm{i}tH}\mathscr{D} \subset \mathscr{D}$ for all $t \in \mathbb{R}$, then it is a core for H. A special instance of such a $\mathscr{D}$ is the set $C^\omega(H)$ of vectors u with the property that the continuous function $u(t) \equiv \mathrm{e}^{\mathrm{i}tH}u$ has an entire analytic extension $\mathbb{C} \ni z \mapsto u(z) \in \mathscr{H}$. The elements of the dense subspace $C^\omega(H)$ are called entire vectors of the group $\mathrm{e}^{\mathrm{i}tH}$.

If $u \in \mathscr{H}_{\mathrm{ac}}(H)$, it follows from Riemann-Lebesgue's lemma that

$$\mathrm{w}-\lim_{|t| \to \infty} \mathrm{e}^{\mathrm{i}tH} u = 0.$$

The density of $\mathscr{L}_{\text{fin}}(\mathscr{H})$ in $\mathscr{L}^{\infty}(\mathscr{H})$ allows to conclude that if C is a compact operator then

$$\lim_{|t|\to\infty} C\mathrm{e}^{\mathrm{i}tH} P_{\mathrm{ac}}(H)u = 0, \tag{8}$$

for all $u \in \mathscr{H}$.

Unitary groups play a central role in quantum dynamics. In fact, they provide the solution to the Cauchy problem for Schrödinger's time dependent equation

$$\mathrm{i}\partial_t u_t = Hu_t,$$

in the form $u_t = \mathrm{e}^{-\mathrm{i}tH}u_0$. The dynamical properties of solutions to this equation depend on the spectral properties of the generator H, the Hamiltonian of the system. The unitary groups $U(t) = \mathrm{e}^{-\mathrm{i}tH}$ is called propagator of the system.

In this section, we review a few classical results of scattering theory in the Hilbert space framework (see [DG, RS3, Y] for more details). We will return to the subject in more detail in Section 5.4.

Consider two strongly continuous unitary groups: $\mathrm{e}^{-\mathrm{i}tH_0}$ representing the free dynamics of the system and $\mathrm{e}^{-\mathrm{i}tH}$ a perturbation of this free dynamics. We say that the state $u \in \mathscr{H}$ is asymptotically free as $t \to \pm\infty$ if there exists $u_\pm \in \mathscr{H}$ such that

$$\lim_{t\to\pm\infty} \|\mathrm{e}^{-\mathrm{i}tH}u - \mathrm{e}^{-\mathrm{i}tH_0}u_\pm\| = 0. \tag{9}$$

u_- (u_+) is the incoming (outgoing) asymptote of u. The condition (9) is clearly equivalent to any of the two following ones

$$\lim_{t\to\pm\infty} \|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}u - u_\pm\| = 0, \qquad \lim_{t\to\pm\infty} \|\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}u_\pm - u\| = 0. \tag{10}$$

The fundamental problems of scattering theory are: (i) to determine the set of asymptotically free states, i.e., the set of $u \in \mathscr{H}$ for which the limits

$$u_\pm = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}u,$$

exist; (ii) the construction of a scattering operator which maps the incoming asymptote u_- into the corresponding outgoing one u_+.

We remark that if u is an eigenvector of H, then the above limits can only exist if u is also an eigenvector of H_0 with the same eigenvalue. Since the eigenvectors of H have a particularly simple time evolution under the group $\mathrm{e}^{-\mathrm{i}tH}$ (they are stationary states), it is natural to restrict our attention to the subspace $\mathscr{H}_{\mathrm{pp}}(H)^{\perp}$. This motivates the following definition of asymptotic completeness.

Definition 2.1 *Let H_0 and H be two self-adjoint operators on the Hilbert space $\mathscr{H}$.*

(1) *The Møller operators $\Omega^\pm(H,H_0)$ exist if the limits*

$$\Omega^\pm(H,H_0)u = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}P_{ac}(H_0)u, \tag{11}$$

exist for all $u \in \mathscr{H}$. In this case, $\Omega^\pm(H,H_0)$ are clearly bounded operators on $\mathscr{H}$.

(2) *The Møller operators* $\Omega^{\pm}(H,H_0)$ *are complete if*

$$\operatorname{Ran}\Omega^{+}(H,H_0)=\operatorname{Ran}\Omega^{-}(H,H_0)=\mathscr{H}_{\mathrm{ac}}(H).$$

(3) *They are asymptotically complete if*

$$\operatorname{Ran}\Omega^{+}(H,H_0)=\operatorname{Ran}\Omega^{-}(H,H_0)=\mathscr{H}_{\mathrm{pp}}(H)^{\perp}.$$

The logic behind these definitions is the following. If $\Omega^{\pm}(H,H_0)$ exist, then they are partial isometries with initial space $\mathscr{H}_{\mathrm{ac}}(H_0)$ and final space $\operatorname{Ran}(\Omega^{\pm}(H,H_0))$. Since obviously

$$\mathrm{e}^{\mathrm{i}tH}\Omega^{\pm}(H,H_0)=\Omega^{\pm}(H,H_0)\mathrm{e}^{\mathrm{i}tH_0},$$

one easily concludes that $\operatorname{Ran}(\Omega^{\pm}(H,H_0))$ reduces H, that $\Omega^{\pm}(H,H_0)\mathrm{Dom}(H_0)\subset\mathrm{Dom}(H)$ and that the intertwining relation $H\Omega^{\pm}(H,H_0)u=\Omega^{\pm}(H,H_0)H_0u$ holds for all $u\in\mathrm{Dom}(H_0)$. Thus the part of H in $\operatorname{Ran}(\Omega^{\pm}(H,H_0))$ is unitarily equivalent to $H_{0,\mathrm{ac}}$ and hence $\operatorname{Ran}(\Omega^{\pm}(H,H_0))\subset\mathscr{H}_{\mathrm{ac}}(H)$. If $\Omega^{\pm}(H,H_0)$ are complete, then they are unitary as maps from $\mathscr{H}_{\mathrm{ac}}(H_0)$ to $\mathscr{H}_{\mathrm{ac}}(H)$ and it follows from the equivalence of the two relations (10) that

$$\Omega^{\pm}(H,H_0)^{*}u=\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}P_{\mathrm{ac}}(H)u=\Omega^{\pm}(H_0,H)u,$$

i.e., the Møller operators $\Omega^{\pm}(H_0,H)$ also exist and are adjoints to $\Omega^{\pm}(H,H_0)$. Thus any $u\in\mathscr{H}_{\mathrm{ac}}(H)$ has incoming/outgoing asymptotes $u_{\pm}=\Omega^{\pm}(H_0,H)u$. The scattering operator $S: u_{-}\mapsto u_{+}$ is given by

$$S=\Omega^{+}(H_0,H)\Omega^{-}(H,H_0)=\Omega^{+}(H,H_0)^{*}\Omega^{-}(H,H_0),$$

and is unitary on $\mathscr{H}_{\mathrm{ac}}(H_0)$. Finally, if in addition H has empty singular continuous spectrum then asymptotic completeness holds and the set of asymptotically free states is $\mathscr{H}_{\mathrm{ac}}(H)=\mathscr{H}_{\mathrm{pp}}(H)^{\perp}$.

The basic method for showing the existence of the Møller operators $\Omega^{\pm}(H,H_0)$ is due to Cook. It is based on the fact that if a function f is differentiable and if $f'\in L^1(\mathbb{R})$, then

$$\lim_{t\to\pm\infty}f(t)=f(0)\pm\int_0^{\infty}f'(\pm t)\,\mathrm{d}t.$$

We thus have that

$$\Omega^{\pm}(H,H_0)u=u\pm\mathrm{i}\int_0^{\infty}\mathrm{e}^{\pm\mathrm{i}tH}(H-H_0)\mathrm{e}^{\mp\mathrm{i}tH_0}u\,\mathrm{d}t,$$

if $\|(H-H_0)\mathrm{e}^{\mp\mathrm{i}tH_0}u\|$ is integrable. This representation is the starting point of many techniques used in scattering theory. In particular, if one can decompose $H-H_0=\sum_j B_j^{*}A_j$, then the Cook representation can we rewritten as

$$(v,\Omega^{\pm}(H,H_0)u)=(v,u)\pm\mathrm{i}\sum_j\int_0^{\infty}(B_j\mathrm{e}^{\mp\mathrm{i}tH}v,A_j\mathrm{e}^{\mp\mathrm{i}tH_0}u)\,\mathrm{d}t,$$

and the Cauchy-Schwarz inequality naturally leads to Kato's definition of smooth perturbation. A closed operator A is called H-smooth if there exists a constant C such that

$$\int_{-\infty}^{\infty} \|A\mathrm{e}^{\mathrm{i}tH} u\|^2 \,\mathrm{d}t \leq C\|u\|^2,$$

for all $u \in \mathscr{H}$. Smoothness is easily localized w.r.t. the spectrum of H: A is said to be H-smooth on the measurable subset $\Delta \subset \mathbb{R}$ if the operator $A1_\Delta(H)$ is H-smooth. If $\mathrm{Dom}(H) \subset \mathrm{Dom}(A)$ and

$$\sup_{\mathrm{Re}\,(z)\in\Delta, \mathrm{Im}\,(z)\neq 0} \|A(H-z)^{-1}A^*\| < \infty, \tag{12}$$

then A is H-smooth on Δ^{cl}.

2.2 C^*-Algebras

In statistical mechanics it is often useful, and sometimes necessary, to consider infinitely extended systems with an infinite number of (classical) degrees of freedom. This is commonly referred to as the *thermodynamic limit.* This is the case, for example, for the construction of nonequilibrium steady states (NESS): in a confined system with a finite number of degrees of freedom there is no dissipative mechanism which would allow it to approach a steady state. In more technical terms, the spectrum of the Hamiltonian H of a confined system is purely discrete and hence its propagator $\mathrm{e}^{\mathrm{i}tH}$ is an almost-periodic function of time which implies that the dynamics is recurrent.

In quantum mechanics, the structure of the algebra of observables of a system with a finite number of degrees of freedom essentially determines the Hilbert space in which these observables are represented by operators (this is the content of the Stone-von Neumann theorem, see theorem VIII.14 in [RS1]). This is the main reason why one generally ignores the algebraic structure of observables in such systems, and instead focuses attention on describing the associated Hilbert space. The situation is completely different when one considers systems with an infinite number of degrees of freedom. Such systems allow for many inequivalent representations and as such, it is necessary to precisely describe the algebra of observables. The mathematical framework necessary for implementing such an algebraic approach to quantum mechanics are operator algebras. Among the different operator algebras, C^*-algebras are particularly well suited for the fermionic systems in which we are interested. In this section, we introduce the basic concepts of the theory of C^*-algebras and their representations. This material is treated in detail in [BR1, BR2].

2.2.1 Definition and examples

Definition 2.2 *(i) A $*$-algebra $\mathscr{A}$ is a complex algebra equipped with an involution $A \mapsto A^*$ such that*

$$(A+B)^* = A^* + B^*, \quad (\lambda A)^* = \overline{\lambda} A^*, \quad (AB)^* = B^* A^*,$$

for all $A, B \in \mathscr{A}$ and $\lambda \in \mathbb{C}$.

(ii) *A Banach algebra $\mathscr{B}$ is a complex algebra such that the underlying vector space is a Banach space with a norm satisfying*

$$\|AB\| \le \|A\|\,\|B\|,$$

for all $A, B \in \mathscr{B}$.

(iii) *A B^*-algebra $\mathscr{B}$ is a Banach algebra as well as a $*$-algebra such that $\|A^*\| = \|A\|$ for all $A \in \mathscr{B}$.*

(iv) *A C^*-algebra $\mathscr{C}$ is a B^*-algebra with a norm satisfying the C^*-property*

$$\|A^*A\| = \|A\|^2,$$

for all $A \in \mathscr{C}$.

Examples of C^*-algebras

1. $\mathscr{A} = \mathscr{B}(\mathscr{H})$, the algebra of bounded operators on a Hilbert space $\mathscr{H}$. In this case, the involution is the operation of adjunction, and the norm is the usual operator norm $\|A\| = \sup\{\|A\psi\| \,|\, \psi \in \mathscr{H}, \|\psi\| = 1\}$. To verify the C^* property of the norm, note that

$$\|A\|^2 = \sup_{\|\psi\|=1} (A\psi, A\psi) = \sup_{\|\psi\|=1} (\psi, A^*A\psi) \le \|A^*A\| \le \|A^*\|\|A\| = \|A\|^2.$$

2. $\mathscr{A} = \mathscr{L}^\infty(\mathscr{H})$, the algebra of compact operators on a Hilbert space $\mathscr{H}$, is a C^*-subalgebra of $\mathscr{B}(\mathscr{H})$ (and a closed two-sided ideal of the latter).

3. $\mathscr{A} = C_\infty(X)$, the algebra of continuous functions on a locally compact space X which vanish at infinity, that is to say the set of all continuous functions $f : X \to \mathbb{C}$ such that, for any $\epsilon > 0$, there exists a compact $K \subset X$ with $|f(x)| < \epsilon$ for all $x \in X \setminus K$. The involution in this case is complex conjugation and the norm is $\|f\| = \sup_{x\in X} |f(x)|$. Let μ be a regular Borel measure on X such that $\mu(O) > 0$ for every open $O \subset X$. By identifying $f \in C_\infty(X)$ with the operator of multiplication by f in the Hilbert space $\mathscr{H} = L^2(X, \mathrm{d}\mu)$, the algebra $C_\infty(X)$ can be viewed as a commutative C^*-subalgebra of $\mathscr{B}(\mathscr{H})$.

4. A subset $\mathscr{S}$ of a $*$-algebra is called self-adjoint if $A \in \mathscr{S}$ implies $A^* \in \mathscr{S}$. Thus, a subalgebra of a $*$-algebra is a $*$-algebra if and only if it is self-adjoint. It follows that a subalgebra of a B^*-algebra (resp. C^*-algebra) is itself a B^*-algebra (resp. C^*-algebra) if and only if it is closed and self-adjoint.

Example 1 is in some sense the most general. More precisely, any C^*-algebra is isomorphic to a subalgebra of $\mathscr{B}(\mathscr{H})$ for some $\mathscr{H}$. A unit in a C^*-algebra $\mathscr{A}$ is a unit for the product operation of $\mathscr{A}$. Such and element, $\mathbb{1}$, if it exists, is unique and satisfies $\mathbb{1}^* = \mathbb{1}$. However, a C^*-algebra does not necessarily contain a unit. For example, the algebra $C_\infty(X)$ has a unit if and only if X is compact and the algebra $\mathscr{L}^\infty(\mathscr{H})$ of all compact operators on the Hilbert space $\mathscr{H}$ has a unit if and only if $\mathscr{H}$ is finite dimensional. The absence of a unit can complicate the structural analysis of $\mathscr{A}$. One can avoid such complications by embedding $\mathscr{A}$ into a larger C^*-algebra $\tilde{\mathscr{A}}$ which contains a unit. The following result describes the canonical construction of this extension.

Proposition 2.3 *Let $\mathscr{A}$ be a C^*-algebra without a unit and $\tilde{\mathscr{A}} = \{\langle \alpha, A\rangle \mid \alpha \in \mathbb{C}, A \in \mathscr{A}\}$ equipped with the operations $\langle \alpha, A\rangle + \langle \beta, B\rangle = \langle \alpha+\beta, A+B\rangle$, $\langle \alpha, A\rangle\langle \beta, B\rangle = \langle \alpha\beta, \alpha B+\beta A+AB\rangle$, $\langle \alpha, A\rangle^* = \langle \overline{\alpha}, A^*\rangle$. It follows that the function*

$$\|\langle \alpha, A\rangle\| = \sup\{\|\alpha B + AB\|, B \in \mathscr{A}, \|B\| = 1\},$$

is a C^*-algebra norm. The algebra $\mathscr{A}$ is identified with the C^*-subalgebra of $\tilde{\mathscr{A}}$ formed by the pairs $\langle 0, A\rangle$ and the element $\langle 1, 0\rangle$ is a unit of $\tilde{\mathscr{A}}$.

The majority of C^*-algebras that appear in quantum physics are naturally equipped with a unit. In the following we will assume, without explicit mention, that all the C^*-algebras contain a unit $\mathbb{1}$.

A $*$-morphism between two $*$-algebras $\mathscr{A}$ and $\mathscr{B}$ is a mapping $\phi : \mathscr{A} \to \mathscr{B}$ which satisfies

(i) $\phi(\alpha A + \beta B) = \alpha\phi(A) + \beta\phi(B)$,

(ii) $\phi(AB) = \phi(A)\phi(B)$,

(iii) $\phi(A^*) = \phi(A)^*$,

for all $A, B \in \mathscr{A}$, $\alpha, \beta \in \mathbb{C}$. A bijective $*$-morphism is called a $*$-isomorphism. A $*$-isomorphism from $\mathscr{A}$ onto itself is called a $*$-automorphism.

2.2.2 Spectral theory

An element A of a C^*-algebra $\mathscr{A}$ is invertible if there exists an element $A^{-1} \in \mathscr{A}$ such that

$$A^{-1}A = AA^{-1} = \mathbb{1}.$$

These elements form a group (w.r.t. the product operation of $\mathscr{A}$), called the group of units of $\mathscr{A}$. We call

$$\mathrm{Res}(A) \equiv \{z \in \mathbb{C} \mid (z\mathbb{1} - A) \text{ is invertible}\},$$

the resolvent set of A and

$$\mathrm{Sp}(A) \equiv \mathbb{C} \setminus \mathrm{Res}(A),$$

the spectrum of A. If $\mathscr{C} \subset \mathscr{A}$ is a C^*-subalgebra and $C \in \mathscr{C}$, the spectrum of C, when regarded as an element of A, coincides with its spectrum when it is regarded as an element of $\mathscr{C}$. In particular, if $\mathscr{A}$ is a C^*-subalgebra of $\mathscr{B}(\mathscr{H})$, the notions of resolvent set and spectrum coincide with those introduced in Section 2.1.1. For all $A \in \mathscr{A}$ we have

(i) $\mathrm{Sp}(A^*) = \overline{\mathrm{Sp}(A)}$.

(ii) $\mathrm{Sp}(A^{-1}) = \mathrm{Sp}(A)^{-1}$.

(iii) $\mathrm{Sp}(P(A)) = P(\mathrm{Sp}(A))$ for any polynomial P.

(iv) $\mathrm{Sp}(AB) \cup \{0\} = \mathrm{Sp}(BA) \cup \{0\}$ for all $B \in \mathscr{A}$.

If $|z| > \|A\|$ then the series

$$\frac{1}{z}\sum_{n\in\mathbb{N}}\left(\frac{A}{z}\right)^n,$$

is norm convergent. Its sum is $(z\mathbb{1} - A)^{-1}$, which implies that $\mathrm{Sp}(A) \subset \{z \in \mathbb{C} \,|\, |z| \le \|A\|\}$. Also, if $A \in \mathscr{A}$ is invertible, and if $\|B - A\|\,\|A^{-1}\| < 1$ then B is invertible, and the series

$$B^{-1} = \sum_{n\in\mathbb{N}} A^{-1}\left((B-A)A^{-1}\right)^n,$$

converges in norm. The group of units of $\mathscr{A}$ is thus open in $\mathscr{A}$ and the mapping $A \mapsto A^{-1}$ is continuous. In particular, if $z_0 \in \mathrm{Res}(A)$, then

$$\{z \in \mathbb{C} \,|\, |z - z_0| < ||(z_0\mathbb{1} - A)^{-1}||^{-1}\} \subset \mathrm{Res}(A),$$

and the series

$$(z\mathbb{1} - A)^{-1} = \sum_{n\in\mathbb{N}} (z_0 - z)^n (z_0\mathbb{1} - A)^{-n-1},$$

converges in norm. We can deduce that:

(i) $\mathrm{Res}(A)$ is open;

(ii) the mapping $z \mapsto (z\mathbb{1} - A)^{-1}$ is analytic on $\mathrm{Res}(A)$;

(iii) $\mathrm{Sp}(A)$ is compact.

We call

$$r(A) \equiv \sup\{|\lambda| \,|\, \lambda \in \mathrm{Sp}(A)\},$$

the spectral radius of A. We have already noted that $r(A) \le \|A\|$. We also have that

$$r(A) = \lim_n ||A^n||^{1/n} = \inf_n ||A^n||^{1/n}.$$

An element A of a C^*-algebra $\mathscr{A}$ is

(i) normal if $A^*A = AA^*$;

(ii) self-adjoint if $A = A^*$;

(iii) positive if $A = A^*$ and $\mathrm{Sp}(A) \subset [0, \infty[$;

(iv) isometric if $A^*A = \mathbb{1}$;

(v) unitary if $A^* A = AA^* = \mathbb{1}$.

If A is normal, then $r(A) = ||A||$. If A is self-adjoint, then $\mathrm{Sp}(A) \subset [-||A||, ||A||]$. If A is isometric, then $r(A) = 1$, and if it is unitary, then $\mathrm{Sp}(A) \subset \{z \in \mathbb{C} \,|\, |z| = 1\}$. If A is positive, we write $A \geq 0$. By writing $A \geq B$ when $A - B \geq 0$ we introduce a partial order on $\mathscr{A}$. For the self-adjoint elements of $\mathscr{A}$, the spectral theorem from Section 2.1.2 can be formulated as follows.

Theorem 2.4 *Let A be a self-adjoint element of the C^*-algebra $\mathscr{A}$ and $C(\mathrm{Sp}(A))$ denote the C^*-algebra of continuous functions on $\mathrm{Sp}(A)$. There exists a unique $*$-morphism*

$$\begin{array}{rcl} C(\mathrm{Sp}(A)) & \to & \mathscr{A} \\ f & \mapsto & f(A), \end{array}$$

that sends the function 1 to $\mathbb{1}$ and the function $\mathrm{Id}_{\mathrm{Sp}(A)}$ to A. Furthermore, we have that

$$\mathrm{Sp}(f(A)) = f(\mathrm{Sp}(A)),$$

for all $f \in C(\mathrm{Sp}(A))$.

Applying this result to the functions $f_\pm(x) = (|x| \pm x)/2$, we obtain that any self-adjoint $A \in \mathscr{A}$ can be written as $A = A_+ - A_-$ where $A_\pm = f_\pm(A) \in \mathscr{A}$ are both positive. Since any $A \in \mathscr{A}$ can be written as $A = X + \mathrm{i}Y$ where both $X = (A + A^*)/2$ and $Y = (A - A^*)/2\mathrm{i}$ are self-adjoint elements of $\mathscr{A}$, we conclude that any $A \in \mathscr{A}$ is a linear combination of 4 positive elements of $\mathscr{A}$.

2.2.3 Representations and states

In this section we discuss two key concepts of the theory of C^*-algebras: representations and states.

Representations. A $*$-morphism ϕ between two C^*-algebras preserves positivity. If $A \geq 0$, we have that $A = B^* B$ for some operator B and thus

$$\phi(A) = \phi(B^* B) = \phi(B)^* \phi(B) \geq 0.$$

ϕ is also continuous and satisfies $||\phi(A)|| \leq ||A||$ for all $A \in \mathscr{A}$. ϕ is injective if and only if one of the following conditions is satisfied.

(i) $\mathrm{Ker}\,\phi = \{0\}$,

(ii) $||\phi(A)|| = ||A||$ for all $A \in \mathscr{A}$,

(iii) $A > 0$ implies $\phi(A) > 0$ for all $A \in \mathscr{A}$.

In particular, every $*$-automorphism of a C^*-algebra is isometric.

Definition 2.5 *A representation of a C^*-algebra $\mathscr{A}$ is a pair $\langle\mathscr{H},\Pi\rangle$ where $\mathscr{H}$ is a Hilbert space and $\Pi:\mathscr{A}\to\mathscr{B}(\mathscr{H})$ is a $*$-morphism. A representation is called faithful if Π is injective.*

Let $\langle\mathscr{H},\Pi\rangle$ be a representation of a C^*-algebra $\mathscr{A}$ and let $\mathscr{H}_1\subset\mathscr{H}$ be a closed, Π-invariant subspace, that is to say that $\Pi(A)\mathscr{H}_1\subset\mathscr{H}_1$ for all $A\in\mathscr{A}$. Let P_1 be the orthogonal projection onto $\mathscr{H}_1$. For all $A\in\mathscr{A}$, we have that $\Pi(A)P_1=P_1\Pi(A)P_1$, and by taking the adjoint, $P_1\Pi(A)=P_1\Pi(A)P_1$. We can then deduce that $\Pi(A)P_1=P_1\Pi(A)$, i.e. P_1 commutes with $\Pi(\mathscr{A})$. Conversely, if an orthogonal projection commutes with $\Pi(\mathscr{A})$, then its range is Π-invariant. This is the case of $P_2=I-P_1$, from which we deduce that $\mathscr{H}_2\equiv\mathscr{H}_1^{\perp}$ is Π-invariant. By writing $\Pi_i(A)=\Pi(A)|_{\mathscr{H}_i}$, we obtain two representations $\langle\mathscr{H}_i,\Pi_i\rangle$ of $\mathscr{A}$ and the decomposition

$$\langle\mathscr{H},\Pi\rangle=\langle\mathscr{H}_1,\Pi_1\rangle\oplus\langle\mathscr{H}_2,\Pi_2\rangle.$$

More generally, for each orthogonal decomposition $\mathscr{H}=\oplus_\alpha\mathscr{H}_\alpha$ into Π-invariant subspaces, we associate the decomposition $\Pi=\oplus_\alpha\Pi_\alpha$.

A representation of a C^*-algebra is called trivial when $\Pi=0$. A representation $\langle\mathscr{H},\Pi\rangle$ can be non-trivial but still have a trivial part $\mathscr{H}_0$ defined by

$$\mathscr{H}_0\equiv\{\psi\in\mathscr{H}\,|\,\Pi(A)\psi=0,\ \ \forall A\in\mathscr{A}\}.$$

A representation is called non-degenerate if $\mathscr{H}_0=\{0\}$.

Two representations $\langle\mathscr{H}_1,\Pi_1\rangle$ and $\langle\mathscr{H}_2,\Pi_2\rangle$ are called equivalent if there exists a unitary $U:\mathscr{H}_1\to\mathscr{H}_2$ such that $U\Pi_1(A)=\Pi_2(A)U$ for all $A\in\mathscr{A}$.

In the next subsection, we will investigate the concept of a state, which plays an important role in the construction of representations.

States. A linear functional ω on a $*$-algebra $\mathscr{A}$ is positive if $\omega(A^*A)\geq 0$ for all $A\in\mathscr{A}$. In this case, $\langle A,B\rangle\mapsto\omega(A^*B)$ is a positive Hermitian form on $\mathscr{A}\times\mathscr{A}$. We deduce that $\omega(A^*B)=\overline{\omega(B^*A)}$ and the Cauchy-Schwarz inequality $|\omega(A^*B)|^2\leq\omega(A^*A)\omega(B^*B)$ holds for all $A,B\in\mathscr{A}$. In particular, if $\mathscr{A}$ has a unit $\mathbb{1}$, then $\omega(A^*)=\overline{\omega(A)}$ and $|\omega(A)|^2\leq\omega(A^*A)\omega(\mathbb{1})$.

A linear functional ω on a C^*-algebra $\mathscr{A}$ is positive if and only if it is continuous and $||\omega||=\omega(\mathbb{1})$. If ω is a positive linear functional on the C^*-algebra $\mathscr{A}$ and $A\in\mathscr{A}$ then $\omega_A(B)\equiv\omega(A^*BA)$ defines a positive linear functional on $\mathscr{A}$ and $|\omega(A^*BA)|\leq\omega(A^*A)||B||$ for all $A,B\in\mathscr{A}$.

A state on a C^*-algebra $\mathscr{A}$ is a positive linear functional normalized by the condition $||\omega||=\omega(\mathbb{1})=1$. The set $E(\mathscr{A})$ of all states on $\mathscr{A}$ is clearly convex. If $\mathscr{A}$ contains a unit then $E(\mathscr{A})$ is a weakly-$*$ compact subset of the topological dual of $\mathscr{A}$.

We recall that a point x of a convex set K is extremal whenever $x=\lambda a+(1-\lambda)b$ with $a,b\in K$ and $\lambda\in]0,1[$ implies $a=b=x$, i.e., x cannot be decomposed in a convex combination of other points of K. The extremal points of $E(\mathscr{A})$ are called pure states.

Cyclic representations. Let $\langle\mathscr{H},\Pi\rangle$ be a representation of the C^*-algebra $\mathscr{A}$. A vector $\Omega\in\mathscr{H}$ is called cyclic for Π if the subspace $\Pi(\mathscr{A})\Omega$ is dense in $\mathscr{H}$. The representation $\langle\mathscr{H},\Pi\rangle$ is cyclic if it admits a cyclic vector. A cyclic representation is non-degenerate. Conversely, every non-degenerate representation $\langle\mathcal{H},\Pi\rangle$ can be decomposed into cyclic representations $\langle\mathcal{H},\Pi\rangle = \oplus_\alpha\langle\mathcal{H}_\alpha,\Pi_\alpha\rangle$.

If $\langle\mathcal{H},\Pi\rangle$ is non-degenerate and $\Omega\in\mathcal{H}$ is a unit vector, then the formula

$$\omega_\Omega(A) = (\Omega,\Pi(A)\Omega),$$

defines a state ω_Ω on $\mathscr{A}$. The following theorem shows that all states on $\mathscr{A}$ are of this form.

Theorem 2.6 (Gelfand, Naimark, Segal) *Let ω be a state on the C^*-algebra $\mathscr{A}$. There exists a cyclic representation $\langle\mathcal{H}_\omega,\Pi_\omega,\Omega_\omega\rangle$ of $\mathscr{A}$ such that for all $A\in\mathscr{A}$:*

$$\omega(A) = (\Omega_\omega,\Pi_\omega(A)\Omega_\omega),$$

with $||\Omega_\omega||^2 = ||\omega|| = 1$. Furthermore, this representation is unique up to a unitary transformation.

We call $\langle\mathcal{H}_\omega,\Pi_\omega,\Omega_\omega\rangle$ the GNS representation, or the canonical cyclic representation of $\mathscr{A}$ associated with ω. It plays a very important role in quantum mechanics because it allows us to associate a Hilbert space framework to a state and to distinguish an important class of states associated with ω. A trace class operator ρ such that $\rho\geq 0$ and $\mathrm{tr}\rho = 1$ is called a density matrix. To each density matrix $\rho\in\mathscr{L}^1(\mathcal{H}_\omega)$ we may associate a state $\omega_\rho\in E(\mathscr{A})$ defined by

$$\omega_\rho(A) = \mathrm{tr}_{\mathcal{H}_\omega}(\rho\Pi_\omega(A)).$$

Such a state is called ω-normal. We denote by $\mathcal{N}_\omega(\mathscr{A})$ the subset of $E(\mathscr{A})$ formed by all ω-normal states. We note that the set of vector states $\omega_\Psi(A) = (\Psi,\Pi_\omega(A)\Psi)$ associated to unit vectors $\Psi\in\mathcal{H}_\omega$ is dense in $\mathcal{N}_\omega(\mathscr{A})$.

2.2.4 C^*-dynamics

A C^*-dynamics on a C^*-algebra $\mathscr{A}$ is a strongly continuous group $\mathbb{R}\ni t\mapsto\tau^t$ of $*$-automorphisms of $\mathscr{A}$, that is to say that for all $t\in\mathbb{R}$, τ^t is a $*$-automorphism of $\mathscr{A}$, such that for all $A\in\mathscr{A}$ the mapping $t\mapsto\tau^t(A)$ is continuous, $\tau^0 = \mathrm{Id}$, and for all $t,s\in\mathbb{R}$, $\tau^t\circ\tau^s = \tau^{t+s}$. The general theory of strongly continuous groups on Banach spaces shows that for all A in a dense subspace $\mathrm{Dom}(\delta)\subset\mathscr{A}$, the limit

$$\delta(A) = \lim_{t\to 0}\frac{\tau^t(A)-A}{t},$$

exists and defines a closed operator on $\mathscr{A}$. The algebraic structure of $\mathscr{A}$ implies that $\mathrm{Dom}(\delta)$ is a $*$-subalgebra of $\mathscr{A}$ and that

$$\delta(AB) = \delta(A)B + A\delta(B),\qquad \delta(A^*) = \delta(A)^*,\qquad \delta(\mathbb{1}) = 0,$$

for all $A,B\in\mathrm{Dom}(\delta)$. Such an operator δ is called a $*$-derivation on $\mathscr{A}$.

If τ^t is a C^*-dynamics on the C^*-algebra $\mathscr{A}$, there exists a dense $*$-subalgebra $\mathscr{A}_\tau \subset \mathscr{A}$ such that for all $A \in \mathscr{A}_\tau$, the function $t \mapsto \tau^t(A)$ has an entire analytic extension $\mathbb{C} \ni z \mapsto \tau^z(A)$. The elements of $\mathscr{A}_\tau$ are called τ-entire.

Example. Let $\mathscr{H}$ be a Hilbert space and H a bounded self-adjoint operator on $\mathscr{H}$. Then $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$ defines a C^*-dynamics on $\mathscr{B}(H)$. Its generator $\delta(A) = \mathrm{i}[H, A]$ is bounded. We note that the boundedness of H is necessary to ensure the strong continuity of τ^t. This fact is one major obstacle to the use of C^*-algebras in quantum mechanics. However, we shall see in Section 3.1.3 that for fermionic systems it is possible to define a C^*-dynamics even in cases where the Hamiltonian is unbounded. For bosonic systems, it is generally preferable to work with von Neumann algebras which avoid this problem.

C^*-dynamical systems

A C^*-dynamical system is a pair $\langle \mathscr{A}, \tau \rangle$ where $\mathscr{A}$ is a C^*-algebra and τ is a C^*-dynamics on $\mathscr{A}$. In the context of quantum mechanics, the elements of $\mathscr{A}$ describe physical observables and the group τ specifies their time evolution in the Heisenberg picture, $A_t = \tau^t(A)$. A state $\omega \in E(\mathscr{A})$ associates to each observable $A \in \mathscr{A}$ a number $\omega(A)$ which may be interpreted as the quantum mechanical expectation value of the observable A. It is thus natural to identify elements of $E(\mathscr{A})$ with the physical states of quantum mechanics. Since $\omega(A_t) = \omega(\tau^t(A)) = \omega \circ \tau^t(A)$, the evolution of quantum states in the Schrödinger picture is given by $\omega_t = \omega \circ \tau^t$. A state ω is τ-invariant if $\omega \circ \tau^t = \omega$ for all $t \in \mathbb{R}$. The set $E(\mathscr{A}, \tau) \subset E(\mathscr{A})$ of all τ-invariant states is never empty. It is the set of all steady states of the system. A state $\omega \in E(\mathscr{A}, \tau)$ is called τ-ergodic if

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \nu \circ \tau^{\pm t}(A)\, \mathrm{d}t = \omega(A), \tag{13}$$

for all $A \in \mathscr{A}$, $\nu \in \mathscr{N}_\omega(\mathscr{A})$. It is called τ-mixing if

$$\lim_{t \to \infty} \nu \circ \tau^{\pm t}(A) = \omega(A), \tag{14}$$

for all $A \in \mathscr{A}$, $\nu \in \mathscr{N}_\omega(\mathscr{A})$.

2.2.5 KMS states

We saw in the previous section that C^*-dynamical systems provide a mathematical framework for quantum mechanics. In this section, we describe how to characterize thermal equilibrium states in the language of C^*-algebras. We shall content ourselves with a very elementary introduction to the KMS condition. The interested reader should consult Chapter 5 of [BR2] for a more detailed discussion as well as [HHW, BF] for a deeper insight into the algebraic structure induced by equilibrium states.

We consider a N-level quantum system described by a Hamiltonian H on the N-dimensional Hilbert space $\mathscr{H}$. The associated C^*-dynamical system is $\langle \mathscr{B}(\mathscr{H}), \tau \rangle$, where $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$.

The Gibbs-Boltzmann Ansatz for the canonical ensemble a temperature T is the density matrix

$$\rho_\beta = Z_\beta^{-1} \mathrm{e}^{-\beta H},$$

where $\beta = 1/k_B T$, k_B being the Boltzmann constant. The normalization factor $Z_\beta = \mathrm{tr}(\mathrm{e}^{-\beta H})$ is the canonical partition function. The state $\omega \in E(\mathscr{B}(\mathscr{H}))$ corresponding to this density matrix is

$$\omega(A) = Z_\beta^{-1} \mathrm{tr}(\mathrm{e}^{-\beta H} A) = \frac{\mathrm{tr}(\mathrm{e}^{-\beta H} A)}{\mathrm{tr}(\mathrm{e}^{-\beta H})}.$$

The equilibrium correlation function

$$F(A, B; t) \equiv \omega(A\tau^t(B)), \tag{15}$$

is an analytic function of $t \in \mathbb{C}$. The cyclic property of the trace yields the following identity

$$\mathrm{tr}(\mathrm{e}^{-\beta H} A \mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH}) = \mathrm{tr}(\mathrm{e}^{-\beta H} \mathrm{e}^{\mathrm{i}(t-\mathrm{i}\beta)H} B \mathrm{e}^{-\mathrm{i}(t-\mathrm{i}\beta)H} A),$$

from which we conclude that

$$F(A, B; t + \mathrm{i}\beta) = \omega(\tau^t(B)A). \tag{16}$$

The relations (15) and (16) represent the values of the analytic function $F(A, B; z)$ along the boundary of the strip $S_\beta \equiv \{z \in \mathbb{C} \,|\, 0 < \mathrm{Im}z < \beta\}$. These relations are called the Kubo-Martin-Schwinger (KMS) boundary conditions.

Definition 2.7 *Let $\langle \mathscr{A}, \tau\rangle$ be a C^*-dynamical system. $\omega \in E(\mathscr{A})$ is a $\langle\tau, \beta\rangle$-KMS state for a $\beta \geq 0$ if, for all $A, B \in \mathscr{A}$, there exists a function $F(A, B; z)$, analytic on the strip S_β, bounded and continuous on its closure and satisfying the KMS boundary conditions (15) and (16).*

Remarks.
1. A $\langle\tau, 0\rangle$-KMS state is also called tracial since it satisfies the cyclicity condition $\omega(AB) = \omega(BA)$.
2. For $\beta > 0$, a $\langle\tau, \beta\rangle$-KMS state represents the thermodynamic state of a system at temperature $T = (k_B \beta)^{-1}$ where k_B is the Boltzmann constant.
3. $\langle\tau, \beta\rangle$-KMS state for $\beta < 0$ can be defined by a straightforward modification of Definition 2.7. If ω is $\langle\tau^t, \beta\rangle$-KMS and $\gamma \neq 0$ then ω is also $\langle\tau^{\gamma t}, \beta/\gamma\rangle$-KMS. However, there is no simple relation between two KMS states at different temperatures for the same dynamics τ^t.
4. The abstract definition of a KMS state masks its fundamental property: Every $\langle\tau, \beta\rangle$-KMS state with $\beta > 0$ is τ-invariant.
5. In practice, it suffices to check the KMS boundary condition on a large enough subalgebra of $\mathscr{A}$: let $\mathscr{C}$ be a dense $*$-subalgebra of the $*$-algebra $\mathscr{A}_\tau$ of τ-entire elements. If $\omega(A\tau^{\mathrm{i}\beta}(B)) = \omega(BA)$ holds for all $A, B \in \mathscr{C}$ then ω is a $\langle\tau, \beta\rangle$-KMS state.
6. The set of all $\langle\tau, \beta\rangle$-KMS states on $\mathscr{A}$ is obviously a convex subset of $E(\mathscr{A})$. Moreover, this subset is weakly-$*$ closed. If $\mathscr{A}$ contains a unit then any $\langle\tau, \beta\rangle$-KMS state is a convex combination of extremal $\langle\tau, \beta\rangle$-KMS states. These extremal $\langle\tau, \beta\rangle$-KMS states are interpreted

in statistical mechanics as pure thermodynamical phases (see Theorem 5.3.30 in [BR2] for a more precise formulation of this property).

The following example shows that KMS states of quantum systems with a finite number of degrees of freedom coincide with the usual notion of equilibrium states from statistical mechanics.

Example: Finite quantum systems. Let H be a self-adjoint operator on the finite-dimensional Hilbert space $\mathscr{H}$. We consider the C^*-dynamical system $\langle \mathscr{B}(\mathscr{H}), \tau\rangle$ where $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$. Any state on $\mathscr{B}(\mathscr{H})$ is of the form $\omega(A) = \mathrm{tr}(\rho A)$ where ρ is a density matrix on $\mathscr{H}$. Suppose that the state defined by the density matrix ρ is $\langle \tau, \beta\rangle$-KMS. The relations (15), (16) applied to $A \equiv \phi(\psi, \cdot)$ give

$$(\psi, \tau^{\mathrm{i}\beta}(B)\rho\phi) = (\psi, \rho B\phi).$$

Since this holds for all $\psi, \phi \in \mathscr{H}$ we must have $\mathrm{e}^{-\beta B} B \mathrm{e}^{\beta H}\rho = \rho B$ for all $B \in \mathscr{B}(\mathscr{H})$. Setting $B \equiv \phi(\psi, \cdot)$ we further obtain

$$\rho\phi = \frac{(\mathrm{e}^{\beta H}\psi, \rho\psi)}{(\psi, \psi)} \mathrm{e}^{-\beta H}\phi,$$

from which we conclude that $\rho = Z_\beta^{-1}\mathrm{e}^{-\beta H}$. Thus the C^*-dynamical system $\langle \mathscr{B}(\mathscr{H}), \tau\rangle$ admits a unique $\langle \tau, \beta\rangle$-KMS state and this state is given by the Gibbs-Boltzmann formula.

2.2.6 Perturbation theory

Time-dependent perturbation theory is an essential tool in the construction of quantum dynamical systems. As far as C^*-dynamics are concerned, it is fairly elementary application of well known techniques. However, the discussion of the KMS states of perturbed dynamical system due to Araki [A3] (see also [BR2, DJP]) which we summarize in this section is more subtle and has important application in equilibrium as well as non-equilibrium statistical mechanics.

Le $\langle \mathscr{A}, \tau\rangle$ be a C^*-dynamical system and denote by δ the $*$-derivation generating the group τ. For any self-adjoint $V \in \mathscr{A}$,

$$\delta_V = \delta + \mathrm{i}[V, \cdot],$$

generates a dynamics τ_V^t on $\mathscr{A}$ given by the Schwinger-Dyson expansion

$$\tau_V^t(A) = \tau^t(A) + \sum_{n=1}^{\infty} \int_{0 \le s_1 \le \cdots \le s_n \le t} \mathrm{i}[\tau^{s_1}(V), \mathrm{i}[\tau^{s_2}(V), \cdots \mathrm{i}[\tau^{s_n}(V), \tau^t(A)]\cdots]]\, \mathrm{d}s_1 \cdots \mathrm{d}s_n,$$

which converges in the norm of $\mathscr{A}$ for any $t \in \mathbb{R}$ and $A \in \mathscr{A}$.

Let Γ_V^t denote the solution of the initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_V^t = \mathrm{i}\Gamma_V^t \tau^t(V), \qquad \Gamma_V^0 = I,$$

that is, the time-ordered exponential

$$\Gamma_V^t = I + \sum_{n=1}^{\infty} \mathrm{i}^n \int_{0 \le s_1 \le \cdots \le s_n \le t} \tau^{s_1}(V) \cdots \tau^{s_n}(V)\, \mathrm{d}s_1 \cdots \mathrm{d}s_n,$$

which, for any $t \in \mathbb{R}$, converges towards a unitary element of $\mathscr{A}$. One easily checks that

$$\tau_V^t(A) = \Gamma_V^t \tau^t(A)(\Gamma_V^t)^{-1}, \tag{17}$$

and the cocycle relation

$$\Gamma_V^{t+s} = \Gamma_V^t \tau^t(\Gamma_V^s) \tag{18}$$

are satisfied for all $t, s \in \mathbb{R}$.

If $V \in \mathscr{A}_\tau$, then the function $t \mapsto \Gamma_V^t$ has an entire analytic extension given by the convergent expansion

$$\Gamma_V^z = I + \sum_{n=1}^{\infty} (\mathrm{i}z)^n \int_{0 \le s_1 \le \cdots \le s_n \le 1} \tau^{zs_1}(V) \cdots \tau^{zs_n}(V)\, \mathrm{d}s_1 \cdots \mathrm{d}s_n.$$

It follows that $\Gamma_V^z \in \mathscr{A}_\tau$ and that relations (17) (with $A \in \mathscr{A}_\tau$) and (18) extend to the complex domain. Moreover, the unitarity relation $\Gamma_V^t \Gamma_V^{t*} = I$ extends to $\Gamma_V^z \Gamma_V^{\bar{z}*} = I$, i.e., $(\Gamma_V^z)^{-1} = \Gamma_V^{\bar{z}*}$.

If $\omega \in E(\mathscr{A})$ is a $\langle \tau, \beta \rangle$-KMS state, a simple calculation shows that

$$\omega^V(A) = \frac{\omega(A\Gamma_V^{\mathrm{i}\beta})}{\omega(\Gamma_V^{\mathrm{i}\beta})} = \frac{\omega(\Gamma_V^{\mathrm{i}\beta/2*} A \Gamma_V^{\mathrm{i}\beta/2})}{\omega(\Gamma_V^{\mathrm{i}\beta/2*} \Gamma_V^{\mathrm{i}\beta/2})},$$

satisfies the KMS condition $\omega^V(A\tau_V^{\mathrm{i}\beta}(B)) = \omega^V(BA)$ for any $A, B \in \mathscr{A}_\tau$, and hence ω_V is a $\langle \tau_V, \beta \rangle$-KMS state. Let $\langle \mathscr{H}_\omega, \Pi_\omega, \Omega_\omega \rangle$ denotes the GNS representation of $\mathscr{A}$ induced by ω and set

$$\Omega^V = \frac{\Pi_\omega(\Gamma_V^{\mathrm{i}\beta/2})\Omega_\omega}{\|\Pi_\omega(\Gamma_V^{\mathrm{i}\beta/2})\Omega_\omega\|}.$$

It follows that $\omega^V(A) = (\Omega^V, \Pi_\omega(A)\Omega^V)$ and in particular that $\omega^V \in \mathscr{N}_\omega(\mathscr{A})$.

By approximating an arbitrary self-adjoint $V \in \mathscr{A}$ by a sequence $V_n \in \mathscr{A}_\tau$ one can show (and this is the delicate point in the analysis) that the sequence Ω^{V_n} converges to a vector Ω^V such that $\omega^V(A) = (\Omega^V, \Pi_\omega(A)\Omega^V)$ is $\langle \tau_V, \beta \rangle$-KMS. The map $\omega \mapsto \omega^V$ obtained in this way is a bijection from the set of $\langle \tau, \beta \rangle$-KMS states to the set of $\langle \tau_V, \beta \rangle$-KMS states. Moreover, the set $\{\omega^V \mid V \in \mathscr{A}_\tau, V = V^*\}$ is dense in the set $\mathscr{N}_\omega(\mathscr{A})$ of all ω-normal states.

2.2.7 Liouvilleans and quantum Koopmanism

Given a C^*-dynamical system $\langle \mathscr{A}, \tau \rangle$ and a representation $\Pi : \mathscr{A} \to \mathscr{B}(\mathscr{H})$, we say that the dynamics is unitarily implemented in the Hilbert space $\mathscr{H}$ if there exists a self-adjoint operator

L on $\mathcal{H}$ such that $\Pi(\tau^t(A)) = \mathrm{e}^{\mathrm{i}tL}\Pi(A)\mathrm{e}^{-\mathrm{i}tL}$ holds for all $t \in \mathbb{R}$ and $A \in \mathcal{A}$. Such an implementation allows to reduce a number of dynamical properties of the system $\langle\mathcal{A},\tau\rangle$ to the spectral analysis of the operator L. In this section, we shall see that the unitary implementation of the dynamics always exists in the GNS representation associated to an invariant state. Moreover, if this state is modular (see Definition 2.8 below) then its ergodicity and mixing properties (Eq. (13) and (14)) can be deduced from the spectral properties of the operator L. This is the quantum version of the Koopman approach to the ergodic theory of classical dynamical systems (see, e.g., Section VII.4 in [RS1]).

Let $\langle\mathcal{A},\tau\rangle$ be a C^*-dynamical systems, $\omega \in E(\mathcal{A},\tau)$ and $\langle\mathcal{H}_\omega,\Pi_\omega,\Omega_\omega\rangle$ the induced GNS representation of $\mathcal{A}$. Since Ω_ω is a cyclic vector and $\|\Pi_\omega(\tau^t(A))\Omega_\omega\|^2 = \omega(\tau^t(A^*A)) = \omega(A^*A) = \|\Pi_\omega(A)\Omega_\omega\|^2$, the map

$$\Pi_\omega(\mathcal{A})\Omega_\omega \ni \Pi_\omega(A)\Omega_\omega \mapsto \Pi_\omega(\tau^t(A))\Omega_\omega,$$

is well defined on a dense subspace of $\mathcal{H}_\omega$ and extends to an isometry $U^t : \mathcal{H}_\omega \to \mathcal{H}_\omega$. Observing that $U^tU^s = U^{t+s}$ and $U^0 = I$, we conclude that U^t is a unitary group. Finally it follows from the estimate $\|(U^t - I)\Pi_\omega(A)\Omega_\omega\|^2 = \omega((\tau^t(A)-A)^*(\tau^t(A)-A)) \le \|\tau^t(A)-A\|^2$ and the continuity of the map $t \mapsto \tau^t(A)$ that U^t is strongly continuous. By Stone's theorem, there exists a self-adjoint operator L_ω on $\mathcal{H}_\omega$ such that $U^t = \mathrm{e}^{\mathrm{i}tL_\omega}$. Since $\mathrm{e}^{\mathrm{i}tL_\omega}\Omega_\omega = \Pi_\omega(\tau^t(I))\Omega_\omega = \Omega_\omega$ one has $\Omega_\omega \in \mathrm{Dom}(L_\omega)$ and $L_\omega\Omega_\omega = 0$. The identity

$$\mathrm{e}^{\mathrm{i}tL_\omega}\Pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL_\omega}\Pi_\omega(B)\Omega_\omega = \mathrm{e}^{\mathrm{i}tL\omega}\Pi_\omega(A\tau^{-t}(B))\Omega_\omega = \Pi_\omega(\tau^t(A))\Pi_\omega(B)\Omega_\omega,$$

holds for any $A, B \in \mathcal{A}$. The cyclicity of Ω_ω allows us to conclude that $\mathrm{e}^{\mathrm{i}tL_\omega}\Pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL_\omega} = \Pi_\omega(\tau^t(A))$ for all $A \in \mathcal{A}$. Thus, L_ω implements the dynamics in the GNS representation. Let L be a self-adjoint operator implementing the dynamics τ on $\mathcal{H}_\omega$ and such that $L\Omega_\omega = 0$. It follows that

$$\mathrm{e}^{\mathrm{i}tL}\Pi_\omega(A)\Omega_\omega = \mathrm{e}^{\mathrm{i}tL}\Pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL}\Omega_\omega = \Pi_\omega(\tau^t(A))\Omega_\omega,$$

from which we conclude that $L = L_\omega$. Thus, the operator L_ω is completely and uniquely determined by the two conditions that it implements the dynamics τ on $\mathcal{H}_\omega$ and annihilates the cyclic vector Ω_ω. We shall call L_ω the Liouvillean of the dynamical system $\langle\mathcal{A},\tau,\omega\rangle$.

Definition 2.8 *A state $\omega \in E(\mathcal{A})$ is called modular if there exist a dynamics τ and a $\beta \neq 0$ such that ω is $\langle\tau,\beta\rangle$-KMS.*

By Remark 3 of Section 2.2.5, we can assume that $\beta = 1$. The dynamics σ_ω such that ω is $\langle\sigma_\omega, 1\rangle$-KMS is called the modular group of ω (the convention $\beta = -1$ has been used in the mathematical literature since the works of Tomita and Takesaki [To, Ta]. This convention is however immaterial). The GNS representation induced by a modular state has a rich structure which was unveiled by Haag, Hugenholtz and Winnink [HHW] (following the pioneering works of Araki, Woods and Wyss [AW1, AW2] on the representations of canonical (anti-)commutation relations), and was fully developed by Tomita and Takesaki to the modular theory of von Neumann algebras. We shall only need the following property (see, e.g., [BR1]).

Proposition 2.9 *If ω is a modular state on $\mathscr{A}$ and $\langle\mathscr{H}_\omega, \Pi_\omega, \Omega_\omega\rangle$ the induced GNS representation then the subspace*

$$\Pi_\omega(\mathscr{A})'\Omega_\omega = \{B\Omega_\omega \,|\, B \in \mathscr{B}(\mathscr{H}_\omega), [B, \Pi_\omega(A)] = 0 \text{ for all } A \in \mathscr{A}\},$$

is dense in $\mathscr{H}_\omega$.

Let $\omega \in E(\mathscr{A}, \tau)$ be modular and let L_ω be the Liouvillean implementing the dynamics τ in the GNS representation $\langle\mathscr{H}_\omega, \Pi_\omega, \Omega_\omega\rangle$. For any unit vector $\Psi \in \Pi_\omega(\mathscr{A})'\Omega_\omega$ one has

$$\begin{aligned}
\omega_\Psi(\tau^t(A)) &= (\Psi, \Pi_\omega(\tau^t(A))\Psi) = (B\Omega_\omega, \Pi_\omega(\tau^t(A))B\Omega_\omega)\\
&= (B^*B\Omega_\omega, \Pi_\omega(\tau^t(A))\Omega_\omega) = (B^*B\Omega_\omega, \mathrm{e}^{\mathrm{i}tL_\omega}\Pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL_\omega}\Omega_\omega)\\
&= (B^*B\Omega_\omega, \mathrm{e}^{\mathrm{i}tL_\omega}\Pi_\omega(A)\Omega_\omega),
\end{aligned}$$

for some $B \in \Pi_\omega(\mathscr{A})'$ and it follows that

$$\frac{1}{T}\int_0^T \omega_\Psi(\tau^t(A))\,\mathrm{d}t = \frac{1}{T}\int_0^T (B^*B\Omega_\omega, \mathrm{e}^{\mathrm{i}tL_\omega}\Pi_\omega(A)\Omega_\omega)\,\mathrm{d}t. \tag{19}$$

To evaluate the limit $T \to \infty$ of the right hand side of this identity, let us define the linear map

$$E_T\Phi = \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tL_\omega}\Phi\,\mathrm{d}t,$$

where, due to the strong continuity of the group $\mathrm{e}^{\mathrm{i}tL_\omega}$, we can take the integral in Riemann sense. Since $\|E_T\Phi\| \le \|\Phi\|$, the maps E_T form a uniformly continuous family. For $\Phi \in \mathrm{Dom}(L_\omega)$ one has

$$\mathrm{e}^{\mathrm{i}tL_\omega}L_\omega\Phi = -i\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}tL_\omega}\Phi,$$

so that

$$\lim_{T\to\pm\infty} E_T L_\omega\Phi = \lim_{T\to\pm\infty}\frac{\mathrm{i}}{T}(I - \mathrm{e}^{\mathrm{i}TL_\omega})\Phi = 0.$$

The uniform continuity of the maps E_T allows us to conclude that $\lim_{T\to\pm\infty} E_T\Phi = 0$ holds for all $\Phi \in \mathrm{Ran}\,(L_\omega)^{\mathrm{cl}} = \mathrm{Ker}\,(L_\omega)^\perp$. Since $E_T\Phi = \Phi$ for $\Phi \in \mathrm{Ker}\,(L_\omega)$, one has

$$\mathrm{s}-\lim_{T\to\pm\infty} E_T = P_0(L_\omega),$$

where $P_0(L_\omega)$ denotes the orthogonal projection on $\mathrm{Ker}\,(L_\omega)$ (this is von Neumann's mean ergodic theorem).

Going back to the identity (19), using the fact that $\Omega_\omega \in \mathrm{Ker}\,(L_\omega)$ to write $P_0(L_\omega) = \Omega_\omega(\Omega_\omega, \cdot) + Q$ where Q is the orthogonal projection on $\mathrm{Ker}\,(L_\omega) \ominus \mathbb{C}\Omega_\omega$, we get

$$\begin{aligned}
\lim_{T\to\pm\infty}\frac{1}{T}\int_0^T \omega_\Psi(\tau^t(A))\,\mathrm{d}t &= (B^*B\Omega_\omega, \Omega_\omega)(\Omega_\omega, \Pi_\omega(A)\Omega_\omega) + (B^*B\Omega_\omega, Q\Pi_\omega(A)\Omega_\omega)\\
&= (\Psi, \Psi)(\Omega_\omega, \Pi_\omega(A)\Omega_\omega) + (B^*B\Omega_\omega, Q\Pi_\omega(A)\Omega_\omega)\\
&= \omega(A) + (B^*B\Omega_\omega, Q\Pi_\omega(A)\Omega_\omega).
\end{aligned} \tag{20}$$

If ω is ergodic, then we must have $(B^*B\Omega_\omega, Q\Pi_\omega(A)\Omega_\omega) = 0$ for all $B \in \Pi_\omega(\mathscr{A})'$ and all $A \in \mathscr{A}$. The cyclicity of Ω_ω implies that $QB^*B\Omega_\omega = 0$ for all $B \in \Pi_\omega(\mathscr{A})'$. One easily checks that $\Pi_\omega(\mathscr{A})'$ is a closed self-adjoint subalgebra of $\mathscr{B}(\mathscr{H}_\omega)$, and hence a C^*-algebra (in fact a von Neumann algebra). Since any element of this algebra is a linear combination of positive elements, it follows that $Q\Psi = 0$ for all $\Psi \in \Pi_\omega(\mathscr{A})'\Omega_\omega$. This vectors forming a dense subspace of $\mathscr{H}_\omega$, one finally concludes that $Q = 0$, i.e., $\mathrm{Ker}\,(L_\omega) = \mathbb{C}\Omega_\omega$. Reciprocally, if $\mathrm{Ker}\,(L_\omega) = \mathbb{C}\Omega_\omega$, then $Q = 0$ and we deduce from Eq. (20) that

$$\lim_{T\to\pm\infty} \frac{1}{T}\int_0^T \omega_\Psi(\tau^t(A))\,\mathrm{d}t = \omega(A),$$

for all $\Psi \in \Pi_\omega(\mathscr{A})'\Omega_\omega$. Since $\|\omega_\Psi - \omega_\Phi\| \le 2\|\Psi - \Phi\|$, this extends by density/continuity to all $\Psi \in \mathscr{H}_\omega$. Finally, any density matrix ρ on $\mathscr{H}_\omega$ has a spectral decomposition $\rho = \sum_n p_n \Phi_n(\Phi_n, \cdot)$ with $p_n \in [0,1]$, $\sum_n p_n = 1$ and $\|\Phi_n\| = 1$ so that, by Fubini's theorem

$$\frac{1}{T}\int_0^T \mathrm{tr}_{\mathscr{H}_\omega}\left(\rho\Pi_\omega(\tau^t(A))\right)\mathrm{d}t = \sum_n p_n \frac{1}{T}\int_0^T \omega_{\Phi_n}(\tau^t(A))\,\mathrm{d}t.$$

The dominated convergence theorem allows us to conclude that the right hand side of this identity converges to $\omega(A)$ as $T \to \pm\infty$. In conclusion, we have shown that ω is ergodic if and only if $\mathrm{Ker}\,(L_\omega) = \mathbb{C}\Omega_\omega$.

Invoking similar arguments, one shows that ω is mixing if and only if

$$\lim_{t\to\pm\infty} (\Psi, \mathrm{e}^{\mathrm{i}tL_\omega}\Phi) = (\Psi, \Omega_\omega)(\Omega_\omega, \Phi),$$

holds for $\Psi \in \Pi_\omega(\mathscr{A})'\Omega_\omega$ and $\Phi \in \Pi_\omega(\mathscr{A})\Omega_\omega$. The density of these two subspaces of $\mathscr{H}_\omega$ implies that this is equivalent to

$$\mathrm{w}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tL_\omega} = \Omega_\omega(\Omega_\omega, \cdot).$$

Moreover, the Riemann-Lebesgue lemma implies that this condition is satisfied provided the spectrum of L_ω on the orthogonal complement of $\mathbb{C}\Omega_\omega$ is purely absolutely continuous. We have proven the following:

Proposition 2.10 *Let $\langle\mathscr{A}, \tau\rangle$ be a C^*-dynamical system and denote by $\langle\mathscr{H}_\omega, \Pi_\omega, \Omega_\omega\rangle$ the GNS representation of $\mathscr{A}$ induced by the modular state $\omega \in E(\mathscr{A}, \tau)$. Denote by L_ω the corresponding Liouvillean.*

(i) *ω is ergodic if and only if* $\mathrm{Ker}\,(L_\omega) = \mathbb{C}\Omega_\omega$.

(ii) *ω is mixing if and only if* $\mathrm{w}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tL_\omega} = \Omega_\omega(\Omega_\omega, \cdot)$.

(iii) *If, apart from a simple eigenvalue* 0, *the spectrum of L_ω is purely absolutely continuous, then ω is mixing.*

3 Elements of nonequilibrium quantum statistical mechanics

3.1 Systems of identical particles

3.1.1 Bosons and fermions

In this section we consider a system of n identical particles. In quantum mechanics each one of these particles is described by a separable Hilbert space $\mathfrak{h}$. The observables associated to this particle are the elements of the C^*-algebra $\mathscr{B}(\mathfrak{h})$. The Hilbert space of the entire system is the tensor product $\mathfrak{h}^{\otimes n} = \mathfrak{h} \otimes \cdots \otimes \mathfrak{h}$ and its observables are the elements of the C^*-algebra $\mathscr{B}(\mathfrak{h}^{\otimes n})$.

The natural action of S_n, the permutation group of n objects, given by

$$\pi \cdot (\phi_1 \otimes \cdots \otimes \phi_n) = \phi_{\pi^{-1}(1)} \otimes \cdots \otimes \phi_{\pi^{-1}(n)},$$

for $\pi \in S_n$, $\phi_1, \dots, \phi_n \in \mathfrak{h}$, extends uniquely to a representation $\psi \mapsto \pi \cdot \psi$ of S_n in $\mathfrak{h}^{\otimes n}$. When the n particles are indistinguishable, which is the case if they are identical, the only states that can be realized physically are those that are invariant under this action. In other words, a vector $\psi \in \mathfrak{h}^{\otimes n}$ represent a physical states of a system of n identical particles iff

$$\pi \cdot \psi = \lambda(\pi)\psi,$$

for all $\pi \in S_n$, where $\lambda(\pi)$ is a phase factor ($|\lambda(\pi)| = 1$). Thus, the subspace spanned by ψ carries a one dimensional sub-representation of S_n. They are only two such representations: the trivial ($\lambda^+(\pi) = 1$) and the alternate ($\lambda^-(\pi) = \varepsilon(\pi)$, the sign of π). It is an experimental fact (and the so-called spin-statistic theorem in quantum field theory, see [SW, J, F]) that particles with integer spin (bosons) transform according to the trivial representation while particles with half-integer spin (fermions) transform according to the alternate representation.

To construct the Hilbert space of a system of n bosons/fermions, we introduce the symmetrization operators

$$P_n^\pm : \psi \mapsto \frac{1}{n!} \sum_{\pi \in S_n} \lambda^\pm(\pi)\pi \cdot \psi.$$

One can easily show that these are orthogonal projections and that $\pi \cdot P_n^\pm \psi = \lambda^\pm(\pi) P_n^\pm \psi$ for all $\psi \in \mathfrak{h}^{\otimes n}$, $\pi \in S_n$. The Hilbert space of the system of n bosons/fermions is the subspace

$$\Gamma_n^\pm(\mathfrak{h}) \equiv P_n^\pm \mathfrak{h}^{\otimes n} = \operatorname{Ran} P_n^\pm \subset \mathfrak{h}^{\otimes n}.$$

We note that if $\dim \mathfrak{h} = d < \infty$ then $\dim \Gamma_n^+(\mathfrak{h}) = \frac{d^n}{n!}$, $\dim \Gamma_n^-(\mathfrak{h}) = \binom{d}{n}$ for $n \le d$ and $\Gamma_n^-(\mathfrak{h}) = \{0\}$ for $n > d$.

3.1.2 Fock space

It is often more convenient to work with an indefinite number of particles (this is in fact necessary to describe the grand canonical ensemble). To do so, we set $\Gamma_0^\pm(\mathfrak{h}) \equiv \mathbb{C}$ and we define

$$\Gamma^\pm(\mathfrak{h}) = \bigoplus_{n\in\mathbb{N}} \Gamma_n^\pm(\mathfrak{h}).$$

The vectors of this space are sequences $\Psi = \{\psi_n\}_{n\in\mathbb{N}}$ with $\psi_n \in \Gamma_n^\pm(\mathfrak{h})$ and such that $\|\Psi\|^2 = \sum_n \|\psi_n\|^2 < \infty$. Equipped with the scalar product

$$(\Psi,\Phi) \equiv \sum_{n\in\mathbb{N}} (\psi_n,\phi_n),$$

$\Gamma^\pm(\mathfrak{h})$ is a Hilbert space which we call bosonic/fermionic Fock space over $\mathfrak{h}$. The state associated to the unit vector $\Psi = \{\psi_n\}_{n\in\mathbb{N}} \in \Gamma^\pm(\mathfrak{h})$ is interpreted in the following manner. The probability to find n particles in the system is $\|\psi_n\|^2$ (note that $1 = \|\Psi\|^2 = \sum_n \|\psi_n\|^2$). The vector $\Omega = \{1,0,0,\ldots\}$ thus describes the state in which there are no particles in the system, and is referred to as the *vacuum state.* The vector $\Psi = \{0,\ldots,0,\psi_n,0,\ldots\}$ describes a system with n particles that are in the state associated to ψ_n. In general one can write

$$\Psi = \{\psi_n\}_{n\in\mathbb{N}} = \sum_{n\in\mathbb{N}} \|\psi_n\| \{0,\ldots,0,\psi_n/\|\psi_n\|,0,\ldots\},$$

which is a coherent superposition of states with a definite number of particles. The construction of the Fock space clearly shows that the subspace

$$\Gamma_{\rm fin}^\pm(\mathfrak{h}) \equiv \left\{\Psi = \{\psi_n\}_{n\in\mathbb{N}} \in \Gamma^\pm(\mathfrak{h}) \,\middle|\, \text{the set } \{n\in\mathbb{N}\,|\,\psi_n \neq 0\} \text{ is finite}\right\},$$

is dense in $\Gamma^\pm(\mathfrak{h})$.

3.1.3 Second quantization

For all $f \in \mathfrak{h}$ we define the *creation operator* of a boson/fermion in the state f by

$$\begin{array}{rcl} a_\pm^*(f) : \Gamma_n^\pm(\mathfrak{h}) & \to & \Gamma_{n+1}^\pm(\mathfrak{h}) \\ P_n^\pm \phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n & \mapsto & \sqrt{n+1}P_{n+1}^\pm \phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n \otimes f. \end{array} \tag{21}$$

Apart from the factor $\sqrt{n+1}$, its interpretation is clear. This operator is extended by linearity to the dense subspace $\Gamma_{\rm fin}^\pm(\mathfrak{h})$. An elementary calculation shows that $\Gamma_{\rm fin}^\pm(\mathfrak{h}) \subset \mathrm{Dom}(a_\pm^*(f)^*)$, that $a_\pm^*(f)^*\Omega = 0$ and that

$$a_\pm^*(f)^* P_n^\pm \phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n = \sum_{j=1}^n (\pm 1)^j (f,\phi_j) P_{n-1}^\pm \phi_1 \otimes \cdots \otimes \cancel{\phi_j} \otimes \cdots \phi_n.$$

From this, we deduce that $a_\pm^*(f)$ is closable. We shall use the same notation for its closure and we note that $a_\pm(f) = a_\pm^*(f)^*$ is closed as well. For obvious reason, we call this last operator the

annihilation operator of a boson/fermion in the state f. We note that $f \mapsto a^*_\pm(f)$ is linear but that $f \mapsto a_\pm(f)$ is anti-linear. In the following, $a^\sharp_\pm$ will denote either $a_\pm$ or $a^*_\pm$.
One can easily verify that for all $f, g \in \mathfrak{h}$ the relations

$$[a_\pm(f), a_\pm(g)]_\pm = [a^*_\pm(f), a_\pm(g)^*]_\pm = 0, \quad [a_\pm(f), a^*_\pm(g)]_\pm = (f, g), \tag{$22_\pm$}$$

holds on $\Gamma^\pm_{\rm fin}(\mathfrak{h})$. There $[A, B]_\pm = AB \mp BA$ denotes the commutator/anti-commutator of A and B. These relations play a fundamental role in the quantum mechanics of systems with an infinite number of degrees of freedom. They are known as the canonical commutation/anti-commutation relations (CCR/CAR). The factor of $\sqrt{n+1}$ from definition (21) is there to ensure the validity of these relations.

In the bosonic case, the operators $a^\sharp_+(f)$ are unbounded. Indeed, assuming $a = a_+(f)$ to be bounded, the CCR imply $aa^* = a^*a + \|f\|^2$ and hence $\|a^*\Psi\|^2 = \|a\Psi\|^2 + \|f\|^2$ for all $\Psi \in \Gamma^+(\mathfrak{h})$. From this we conclude that $\|a^*\|^2 = \|a\|^2 + \|f\|^2$ which implies $f = 0$. In the fermionic case, if $a = a_-(f)$ then the CAR imply $a^2 = 0$ and $a^*a\|f\|^2 = a^*[a, a^*]_- a = (a^*a)^2$. We conclude that $\|a\|^2 = \|a^*a\| = \|f\|^2$ and hence $\|a\| = \|a^*\| = \|f\|$. We note in particular that $a^*_-(f)^2 = 0$ shows that it is impossible to create two fermions in the same state. This fundamental property of fermions is known as the Pauli exclusion principle.

Let $T \in \mathscr{B}(\mathfrak{h})$ be a contraction, i.e., $\|T\| \le 1$. We define the operator $\Gamma_n(T)$ acting on $\mathfrak{h}^{\otimes n}$ by the formula $\Gamma_n(T)(\phi_1 \otimes \cdots \otimes \phi_n) = T\phi_1 \otimes \cdots \otimes T\phi_n$. Clearly, $\Gamma_n(T)$ is a contraction which commutes with the projections $P^\pm_n$. Its restriction to $\Gamma^\pm_n(\mathfrak{h})$ is thus a contraction as well as the operator $\Gamma(T) \equiv \oplus_n \Gamma_n(T) : \Gamma^\pm(\mathfrak{h}) \to \Gamma^\pm(\mathfrak{h})$. We say that $\Gamma(T)$ is the second quantization of T. We clearly have that $\Gamma(T)^* = \Gamma(T^*)$ and $\Gamma(TS) = \Gamma(T)\Gamma(S)$. It immediately follows that from definition (21) that $\Gamma(T)a^*_\pm(f) = a^*_\pm(Tf)\Gamma(T)$. By adjunction we obtain $a_\pm(f)\Gamma(T) = \Gamma(T)a_\pm(T^*f)$. If $T \in \mathscr{L}^1(\mathfrak{h})$ is a contraction and if, in the bosonic case, $\|T\|_1 < 1$, then an elementary calculation shows that $\Gamma(T) \in \mathscr{L}^1(\Gamma^\pm(\mathfrak{h}))$ and that we have $\|\Gamma(T)\|_{\Gamma^\pm(\mathfrak{h})} \le \det(I \mp |T|)^{\mp 1}$ and

$$\mathrm{tr}_{\Gamma^\pm(\mathfrak{h})}(\Gamma(T)) = \det(I \mp T)^{\mp 1}. \tag{23}$$

The second quantization of unitary operators is a particularly important case. If U is unitary, then so is $\Gamma(U)$ and we have $\Gamma(U)a^\sharp_\pm(f)\Gamma(U)^* = a^\sharp_\pm(Uf)$. If $U(t) = \mathrm{e}^{\mathrm{i}tH}$ is a strongly continuous unitary group then so is its second quantization. Stone's theorem implies the existence of a self-adjoint operator $\mathrm{d}\Gamma(H)$ on $\Gamma^\pm(\mathfrak{h})$ such that $\Gamma(e^{\mathrm{i}tH}) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(H)}$. The operator $\mathrm{d}\Gamma(H)$ is called the differential second quantization of H. The dense subspace $\Gamma^\pm_{\rm fin}(\mathrm{Dom}(H))$ is a core of $\mathrm{d}\Gamma(H)$ and for all $\Psi = \{\psi_n\}_{n\in\mathbb{N}} \in \Gamma^\pm_{\rm fin}(\mathrm{Dom}(H))$, we have

$$(\mathrm{d}\Gamma(H)\Psi)_n = (H \otimes I \otimes \cdots \otimes I + I \otimes H \otimes \cdots \otimes I + \cdots + I \otimes I \otimes \cdots \otimes H)\psi_n.$$

If both H and A are self-adjoint then

$$\Gamma(\mathrm{e}^{\mathrm{i}tH})\Gamma(\mathrm{e}^{\mathrm{i}sA})\Gamma(\mathrm{e}^{-\mathrm{i}tH}) = \Gamma(\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{\mathrm{i}sA}\mathrm{e}^{-\mathrm{i}tH}) = \Gamma(\mathrm{e}^{\mathrm{i}s\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH}}),$$

which implies $\Gamma(\mathrm{e}^{\mathrm{i}tH})\mathrm{d}\Gamma(A)\Gamma(\mathrm{e}^{-\mathrm{i}tH}) = d\Gamma(\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH})$, and thus $[\mathrm{d}\Gamma(H), \mathrm{d}\Gamma(A)] = \mathrm{d}\Gamma([H, A])$.

3.1.4 The C^*-algebra $\mathrm{CAR}(\mathfrak{h})$

In what follows, we will only consider the fermionic case. To simplify the notation we set $a^\sharp = a^\sharp_-$.

In the fermionic case, the operators $a^\sharp(f)$ being bounded, we can define $\mathrm{CAR}(\mathfrak{h})$ as the C^*-subalgebra of $\mathscr{B}(\Gamma^-(\mathfrak{h}))$ generated by $\{a^\sharp(f) \,|\, f \in \mathfrak{h}\}$. $\mathrm{CAR}(\mathfrak{h}) = \mathscr{B}(\Gamma^-(\mathfrak{h}))$ iff $\mathfrak{h}$ is finite dimensional. One can show that up to a $*$-isomorphism it is the unique C^*-algebra generated by elements $a(f)$ satisfying the canonical anti-commutation relations (23_-). If $\mathfrak{h}$ is infinite dimensional and separable, then $\mathrm{CAR}(\mathfrak{h})$ is also infinite dimensional and separable. If $(e_n)_{n\in N}$ is an orthonormal basis of $\mathfrak{h}$ and $a^\sharp_n \equiv a^\sharp(e_n)$ then the $*$-algebra of all polynomials in $a^\sharp_n$ is dense in $\mathrm{CAR}(\mathfrak{h})$. By using the anti-commutation relations, one can show that $\mathrm{d}\Gamma(f(g,\cdot)) = a^*(f)a(g) \in \mathrm{CAR}(\mathfrak{h})$ for all $f, g \in \mathfrak{h}$. The canonical decomposition of a compact operator allows us to deduce that $\mathrm{d}\Gamma(C) \in \mathrm{CAR}(\mathfrak{h})$ for all $C \in \mathscr{L}^1(\mathfrak{h})$.

If U (resp. V) is a bounded linear (resp. anti-linear) operator on $\mathfrak{h}$ and if $V^*U + U^*V = UV^* + VU^* = 0$ and $U^*U + V^*V = UU^* + VV^* = I$ then there exists a unique $*$-automorphism τ of $\mathrm{CAR}(\mathfrak{h})$ such that $\tau(a(f)) = a(Uf) + a^*(Vf)$ for all $f \in \mathfrak{h}$. We call τ the Bogoliubov automorphism associated wit the pair $\langle U, V\rangle$. In particular, if U is unitary and $V = 0$ the above conditions are satisfied and $\tau(a(f)) = a(Uf)$. If $U(t) = \mathrm{e}^{\mathrm{i}tH}$ is a strongly continuous unitary group on $\mathfrak{h}$, we may thus associate to it a group of Bogoliubov automorphisms $\tau^t_H(a^\sharp(f)) = a^\sharp(\mathrm{e}^{\mathrm{i}tH} f)$. Note that $\tau^t_H(a^\sharp(f)) - a^\sharp(f) = a^\sharp(\mathrm{e}^{\mathrm{i}tH} f - f)$ implies $\|\tau^t_H(a^\sharp(f)) - a^\sharp(f)\| = \|\mathrm{e}^{\mathrm{i}tH} f - f\|$, which shows that $t \mapsto \tau^t_H(a^\sharp(f))$ is continuous. Since τ^t_H is a $*$-morphism, we infer that $t \mapsto \tau^t_H(A)$ is continuous for all polynomials A in $a^\sharp(\cdot)$. Finally, these polynomials being dense in $\mathrm{CAR}(\mathfrak{h})$ and τ^t_H being isometric, we conclude that $t \mapsto \tau^t_H(A)$ is continuous for all $A \in \mathrm{CAR}(\mathfrak{h})$. $\langle \mathrm{CAR}(\mathfrak{h}), \tau_H\rangle$ is a C^*-dynamical system.

3.2 The ideal Fermi gas

The simplest thermodynamic models describe systems of many non-interacting particles, also known as ideal gases. In this section we discuss the ideal Fermi gas which is main object of interest in this notes.

3.2.1 The C^*-dynamical system $\langle \mathrm{CAR}(\mathfrak{h}), \tau_H\rangle$

As seen in the previous section, the Hilbert space of a system of n indistinguishable fermions with one-particle Hilbert space $\mathfrak{h}$ is the completely anti-symmetric tensor product $\Gamma^-_n(\mathfrak{h})$. If the fermions are non-interacting then their Hamiltonian is given by

$$H_n = H \otimes I \otimes \cdots \otimes I + \cdots + I \otimes I \otimes \cdots \otimes H,$$

where H denotes the one-particle Hamiltonian. The propagator of the system is thus

$$U_n(t) = \mathrm{e}^{-\mathrm{i}tH_n} = \Gamma_n(\mathrm{e}^{-\mathrm{i}tH}).$$

It is now easy to describe the system with an indefinite number of fermions. Its Hilbert space is the fermionic Fock space $\Gamma^-(\mathfrak{h}) = \oplus_n \Gamma_n^-(\mathfrak{h})$ and its propagator is the second quantization

$$\Gamma(\mathrm{e}^{-\mathrm{i}tH}) = \oplus_n \Gamma_n(\mathrm{e}^{-\mathrm{i}tH}).$$

Therefore, the time evolution of observables of the system, in the Heisenberg picture, is given by $A_t = \Gamma(\mathrm{e}^{\mathrm{i}tH})A\Gamma(\mathrm{e}^{-\mathrm{i}tH})$. In particular we have $\Gamma(\mathrm{e}^{\mathrm{i}tH})a^\sharp(f)\Gamma(\mathrm{e}^{-\mathrm{i}tH}) = a^\sharp(\mathrm{e}^{\mathrm{i}tH}f) = \tau_H^t(a^\sharp(f))$. We can thus describe an ideal Fermi gas by the C^*-dynamical system $\langle \mathrm{CAR}(\mathfrak{h}), \tau_H^t\rangle$, where $\mathfrak{h}$ is the one-particle Hilbert space and H the one-particle Hamiltonian.

3.2.2 Gauge invariance

Gauge invariance is a fundamental symmetry of quantum mechanics. It arises from the fact that the density matrix $\rho_\phi = \phi(\phi, \cdot)$ which describes the state associated to the vector $\phi \in \mathfrak{h}$ is invariant under the gauge transformation $\phi \mapsto \mathrm{e}^{\mathrm{i}\theta}\phi$. In other words, the phase of the wave function ϕ is not observable. The strongly continuous unitary group $\theta \mapsto \mathrm{e}^{\mathrm{i}\theta I}$ on $\mathfrak{h}$ is called the gauge group. This group is isomorphic to the circle $\mathbb{R}/2\pi\mathbb{Z}$. Gauge invariance is manifest in the Heisenberg picture since observables are invariant under transformations by elements of the gauge group, $\mathrm{e}^{\mathrm{i}\theta I}A\mathrm{e}^{-\mathrm{i}\theta I} = A$ for all $A \in \mathscr{B}(\mathfrak{h})$.

To understand the consequences of this invariance on the algebraic description of the Fermi gas, we note that the gauge group $\mathrm{e}^{\mathrm{i}\theta I}$ induces the unitary group $\Gamma(\mathrm{e}^{\mathrm{i}\theta I})$ in the Fock space $\Gamma^-(\mathfrak{h})$. The generator of this group is the self-adjoint operator $N \equiv \mathrm{d}\Gamma(I)$ which, in the n-particle subspace $\Gamma_n^-(\mathfrak{h})$, acts as multiplication by the number n. N is aptly called the *number operator* and gauge invariance in Fock space expresses the fact that the total number of particles is conserved. The observables of a Fermi gas must be invariant under the action of the gauge group. On the C^*-algebra $\mathrm{CAR}(\mathfrak{h})$, this action is described by the Bogoliubov group

$$\vartheta^\theta(A) = \Gamma(\mathrm{e}^{\mathrm{i}\theta I})A\Gamma(\mathrm{e}^{-\mathrm{i}\theta I}) = \mathrm{e}^{\mathrm{i}\theta N}A\mathrm{e}^{-\mathrm{i}\theta N},$$

which clearly commutes with the dynamical group τ_H^t. We note that the linearity/anti-linearity properties of $f \mapsto a^\sharp(f)$ imply $\vartheta^\theta(a^*(f)) = \mathrm{e}^{\mathrm{i}\theta}a^*(f)$ and $\vartheta^\theta(a(f)) = \mathrm{e}^{-\mathrm{i}\theta}a(f)$. A monomial A in $a^\sharp$ containing n factors of a^* and m factors of a transforms as $\vartheta^\theta(A) = \mathrm{e}^{\mathrm{i}\theta(n-m)}A$. Thus, A is invariant under ϑ iff $n = m$, i.e. iff A preserves the number of fermions. It is evident that a polynomial in $a^\sharp$ is invariant under ϑ if and only if all its monomials terms are invariant themselves. We conclude from this that the gauge invariant C^*-subalgebra

$$\mathrm{CAR}_\vartheta(\mathfrak{h}) \equiv \{A \in \mathrm{CAR}(\mathfrak{h}) \,|\, \vartheta^\theta(A) = A \text{ for all } \theta \in \mathbb{R}\},$$

is the C^*-algebra generated by $\{a^*(f)a(g) \,|\, f, g \in \mathfrak{h}\} \cup \{I\}$. The C^*-dynamical system describing an ideal Fermi gas is thus $\langle \mathrm{CAR}_\vartheta(\mathfrak{h}), \tau_H\rangle$. It is however more convenient to work with the system $\langle \mathrm{CAR}(\mathfrak{h}), \tau_H\rangle$. To do this, one introduces the following notion.

A state $\omega \in E(\mathrm{CAR}(\mathfrak{h}))$ is gauge invariant if it is ϑ-invariant, i.e., $\omega \circ \vartheta^\theta = \omega$ for all $\theta \in \mathbb{R}$.

We then note that $\mathrm{CAR}(\mathfrak{h}) = \oplus_{k\in\mathbb{Z}} \mathrm{CAR}_\vartheta^k(\mathfrak{h})$ where

$$\mathrm{CAR}_\vartheta^k(\mathfrak{h}) \equiv \{A \in \mathrm{CAR}(\mathfrak{h}) \,|\, \vartheta^\theta(A) = \mathrm{e}^{\mathrm{i}k\theta}A \text{ for all } \theta \in \mathbb{R}\},$$

are ϑ-covariant subspaces. Evidently, we have that $\mathrm{CAR}_\vartheta^m(\mathfrak{h})^* = \mathrm{CAR}_\vartheta^{-m}(\mathfrak{h})$ and

$$\mathrm{CAR}_\vartheta^n(\mathfrak{h})\mathrm{CAR}_\vartheta^m(\mathfrak{h}) = \mathrm{CAR}_\vartheta^{n+m}(\mathfrak{h}).$$

If $\omega \in E(\mathrm{CAR}(\mathfrak{h}))$ is gauge invariant one can conclude that $\omega|_{\mathrm{CAR}_\vartheta^k(\mathfrak{h})} = 0$ for $k \neq 0$ while $\omega|_{\mathrm{CAR}_\vartheta(\mathfrak{h})}$ is a state on $\mathrm{CAR}_\vartheta(\mathfrak{h})$. Conversely, a state $\omega \in E(\mathrm{CAR}_\vartheta(\mathfrak{h}))$ extends uniquely to a gauge invariant state on $\mathrm{CAR}(\mathfrak{h})$ by setting $\omega(\oplus_{k\in\mathbb{Z}} A_k) = \omega(A_0)$. There thus exists a bijection between the states of $\mathrm{CAR}_\vartheta(\mathfrak{h})$ and the gauge invariant states of $\mathrm{CAR}(\mathfrak{h})$. The dynamical systems $\langle \mathrm{CAR}_\vartheta(\mathfrak{h}), \tau_H\rangle$ and $\langle \mathrm{CAR}(\mathfrak{h}), \tau_H\rangle$ are clearly equivalent if we restrict the latter one to its gauge invariant states.

3.2.3 $\langle \tau_H, \beta\rangle$-KMS states on $\mathrm{CAR}_\vartheta(\mathfrak{h})$

The first issue which arises naturally after the discussion of the previous section is to characterize the gauge invariant states on $\mathrm{CAR}(\mathfrak{h})$ which correspond to the $\langle \tau_H, \beta\rangle$-KMS states on $\mathrm{CAR}_\vartheta(\mathfrak{h})$. This problem was solved in a very general setting by Araki (see Section 5.4.3 in [BR2]). If ω is an extremal $\langle \tau_H, \beta\rangle$-KMS state on $\mathrm{CAR}_\vartheta(\mathfrak{h})$ with $\beta > 0$ there exists $\mu \in \mathbb{R}$ such that ω is a $\langle \gamma_\mu, \beta\rangle$-KMS state on $\mathrm{CAR}(\mathfrak{h})$, where the C^*-dynamics γ_μ is defined by $\gamma_\mu^t \equiv \tau^t \circ \vartheta^{-\mu t}$. Such a state represents the thermal equilibrium of an ideal Fermi gas at inverse temperature β and at chemical potential μ (*c.f.* Section 3.2.6 below). We note that γ_μ is the Bogoliubov group associated with the operator $K_\mu \equiv H - \mu I$.

We now determine the gauge invariant $\langle \tau_K, \beta\rangle$-KMS states on $\mathrm{CAR}(\mathfrak{h})$, for a self-adjoint operator K on an arbitrary Hilbert space $\mathfrak{h}$. Let ω be such a state. Then, $\langle f, g\rangle \mapsto \omega(a^*(g)a(f))$ is a sesquilinear form on $\mathfrak{h}$. Furthermore

$$0 \le \omega(a^*(f)a(f)) \le \|a^*(f)\|\,\|a(f)\| = \|f\|^2,$$

shows that it is positive and bounded above. Thus, there exists an operator T on $\mathfrak{h}$ such that $0 \le T \le I$ and

$$\omega(a^*(g)a(f)) = (f, Tg). \tag{24}$$

For $t \in \mathbb{R}$ we have $F(t) \equiv \omega(a^*(g)\tau_K^t(a(f))) = (\mathrm{e}^{\mathrm{i}tK} f, Tg)$ and, if $f \in C^\omega(K)$,

$$F(0 + \mathrm{i}\beta) = (\mathrm{e}^{\beta K} f, Tg).$$

The CAR give us that $a(f)a^*(g) = -a^*(g)a(f) + (f, g)$ and thus, taking into account (24),

$$\omega(a(f)a^*(g)) = (f, g) - \omega(a^*(g)a(f)) = (f, (I - T)g).$$

For $t = 0$, the KMS boundary conditions $F(\mathrm{i}\beta) = \omega(a(f)a^*(g))$ imply

$$(\mathrm{e}^{\beta K} f, Tg) = (f, (I - T)g),$$

that is to say $T(I + \mathrm{e}^{\beta K})f = f$ for all $f \in C^\omega(K)$. Since $C^\omega(K)$ is dense and $(I + \mathrm{e}^{\beta K})^{-1} C^\omega(K) \subset C^\omega(K)$ we may deduce that

$$T = (1 + \mathrm{e}^{\beta K})^{-1}. \tag{25}$$

We now consider the function

$$W_{m,n}(g_1,\dots,g_m;f_1,\dots,f_n)=\omega(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)). \tag{26}$$

Gauge invariance implies that $W_{m,n}=0$ if $m\neq n$. If $m=n$, the KMS condition allows us to write

$$W_{n,n}(g_1,\dots,g_n;f_1,\dots,f_n)=\omega(a(\mathrm{e}^{-\beta K}f_n)a^*(g_n)\cdots a^*(g_1)a(f_1)\cdots a(f_{n-1})).$$

By using the CAR, we can bring the first factor on the right hand side to its original position, thus obtaining

$$\begin{aligned}W_{n,n}(g_1,\dots,g_n;f_1,\dots,f_n)&=-W_{n,n}(g_1,\dots,g_n;f_1,\dots,\mathrm{e}^{-\beta K}f_n)\\&\quad+\sum_{j=1}^{n}(-1)^{n+j}(\mathrm{e}^{-\beta K}f_n,g_j)\omega(a^*(g_n)\cdots\cancel{a^*(g_j)}\cdots a^*(g_1)a(f_1)\cdots a(f_{n-1})).\end{aligned}$$

By using the multilinearity of $W_{n,n}$ we can rewrite this identity as

$$\begin{aligned}&W_{n,n}(g_1,\dots,g_n;f_1,\dots,(I+\mathrm{e}^{-\beta K})f_n)\\&\qquad=\sum_{j=1}^{n}(-1)^{n+j}(\mathrm{e}^{-\beta K}f_n,g_j)W_{n-1,n-1}(g_1,\dots,\cancel{g_j},\dots g_n;f_1,\dots,f_{n-1}).\end{aligned}$$

Since $\mathrm{Ran}\,(I+\mathrm{e}^{-\beta K})=\mathfrak{h}$, we may replace f_n by $(I+\mathrm{e}^{-\beta K})^{-1}f_n$ in this last formula to obtain

$$W_{n,n}(g_1,\dots,g_n;f_1,\dots,f_n)=\sum_{j=1}^{n+j}(-1)^{n+j}W_{1,1}(g_j,f_n)W_{n-1,n-1}(g_1,\dots,\cancel{g_j},\dots g_n;f_1,\dots,f_{n-1}).$$

One recognizes this last expression as the Laplace expansion for the determinant of the $n\times n$ matrix $[W_{1,1}(g_j,f_i)]_{i,j=1,\dots,n}$ along the nth row. We are led to conclude that

$$\omega(a^*(g_m)\dots a^*(g_1)a(f_1)\dots a(f_n))=\delta_{n,m}\det[(f_j,Tg_k)].$$

Definition 3.1 *A gauge invariant state $\omega\in E(\mathrm{CAR}(\mathfrak{h}))$ is called quasi-free if there exists a self-adjoint operator T on $\mathfrak{h}$ such that $0\le T\le I$ and*

$$\omega(a^*(g_m)\dots a^*(g_1)a(f_1)\dots a(f_n))=\delta_{n,m}\det[(f_j,Tg_k)]_{j,k=1,\dots,n}, \tag{27}$$

for all $n,m\in\mathbb{N}$ and all $f_1,\dots,f_n,g_1,\dots,g_m\in\mathfrak{h}$. In this case we say that ω is the gauge invariant quasi-free state generated by T and that T is the generator of ω.

Remarks. 1. Since polynomials in $a^\sharp$ are dense in $\mathrm{CAR}(\mathfrak{h})$, it is clear that a state on this C^*-algebra is completely determined by its correlation functions (26).
2. One can show that for any self-adjoint operator T on $\mathfrak{h}$ such that $0\le T\le I$, Formula (27) defines a gauge invariant state on $\mathrm{CAR}(\mathfrak{h})$.
3. If $C\in\mathscr{L}^1(\mathfrak{h})$ we have already noted that $\mathrm{d}\Gamma(C)\in\mathrm{CAR}(\mathfrak{h})$. If $C=\sum_k\kappa_k f_k(g_k,\cdot)$ denotes the canonical decomposition of C, then

$$\mathrm{d}\Gamma(C)=\sum_k\kappa_k\,a^*(f_k)a(g_k),$$

and if $\omega \in E(\mathrm{CAR}(\mathfrak{h}))$ is gauge invariant quasi-free generated by T, then

$$\omega(\mathrm{d}\Gamma(C)) = \sum_k \kappa_k \omega(a^*(f_k)a(g_k)) = \sum_k \kappa_k (g_k, T f_k) = \mathrm{tr}(TC).$$

4. If $\mathfrak{h}$ is finite dimensional, it follows from the final example in Section 2.2.5 and the calculation of this section that

$$\frac{\mathrm{tr}_{\Gamma^-(\mathfrak{h})}(\mathrm{e}^{-\mathrm{d}\Gamma(K)}A)}{\mathrm{tr}_{\Gamma^-(\mathfrak{h})}(\mathrm{e}^{-\mathrm{d}\Gamma(K)})} = \omega_T(A),$$

where ω_T is the gauge invariant quasi-free state generated by $T = (1+\mathrm{e}^K)^{-1}$. Since $\mathrm{e}^{-\mathrm{d}\Gamma(K)} = \Gamma(\mathrm{e}^{-K}) = \Gamma(T(I-T)^{-1})$, Eq. (23) leads to

$$\omega_T(\Gamma(S)) = \frac{\mathrm{tr}_{\Gamma^-(\mathfrak{h})}(\Gamma(T(I-T)^{-1}S)}{\mathrm{tr}_{\Gamma^-(\mathfrak{h})}(\Gamma(T(I-T)^{-1}))} = \frac{\det(I+T(I-T)^{-1}S)}{\det(I+T(I-T)^{-1})} = \det(I+T(S-1)). \tag{28}$$

This formula remains valid for infinite dimensional $\mathfrak{h}$ provided $S-I$ is trace class.
5. The gauge invariant quasi-free state ω_T is modular iff $\mathrm{Ker}\,(T) = \mathrm{Ker}\,(I-T) = \{0\}$. In this case, inverting Eq. (25) yields that the modular group of ω_T is the Bogoliubov group τ_K generated by the Hamiltonian $K = \log\left(T(I-T)^{-1}\right)$.

We thus have the following result

Theorem 3.2 *For all $\beta \in \mathbb{R}$ there exists a unique gauge invariant $\langle \tau_K, \beta\rangle$-KMS state on $\mathrm{CAR}(\mathfrak{h})$. It is the gauge invariant quasi-free state generated by $(1+\mathrm{e}^{\beta K})^{-1}$.*

and its corollary,

Corollary 3.3 *If ω is an extremal $\langle \tau_H, \beta\rangle$-KMS state on $\mathrm{CAR}_\vartheta(\mathfrak{h})$ for $\beta > 0$ there exists $\mu \in \mathbb{R}$ such that ω is the restriction to $\mathrm{CAR}_\vartheta(\mathfrak{h})$ of the gauge invariant quasi-free state on $\mathrm{CAR}(\mathfrak{h})$ generated by $(1+\mathrm{e}^{\beta(H-\mu)})^{-1}$.*

3.2.4 The Araki-Wyss representation

A GNS representation $\langle \mathcal{H}_{\omega_T}, \Pi_{\omega_T}, \Omega_{\omega_T}\rangle$ of $\mathrm{CAR}(\mathfrak{h})$ induced by the gauge invariant quasi-free state ω_T was explicitly constructed by Araki and Wyss in [AW2] (see also [De2]). The Hilbert space is a Fermionic Fock space

$$\mathcal{H}_{\omega_T} = \Gamma^-(\mathfrak{h}\oplus\mathfrak{h}),$$

and the cyclic vector Ω_ω is its the vacuum vector. The morphism $\Pi_\omega : \mathrm{CAR}(\mathfrak{h}) \to \mathcal{B}(\mathcal{H}_\omega)$ is completely determined by

$$\Pi_{\omega_T}(a(f)) = a((I-T)^{1/2}f \oplus 0) + a^*(0 \oplus \overline{T}^{1/2}\overline{f})$$

where $\bar{\cdot}$ denotes an arbitrary complex conjugation on $\mathfrak{h}$ and $\overline{T}$ is defined by $\overline{T}f = \overline{T\overline{f}}$.

If H is a self-adjoint operator on $\mathfrak{h}$ commuting with T and

$$L = \mathrm{d}\Gamma(H \oplus 0 - 0 \oplus \overline{H}),$$

one easily check that

$$\mathrm{e}^{\mathrm{i}tL}\Pi_{\omega_T}(a(f))\mathrm{e}^{-\mathrm{i}tL} = \Pi_{\omega_T}(a(\mathrm{e}^{\mathrm{i}tH}f)),$$

and since $L\Omega_\omega = 0$, we conclude that L is the Liouvillean associated to the Bogoliubov dynamics τ_H. In particular, $\omega_T \in E(\mathrm{CAR}(\mathfrak{h}), \tau_H)$.

If H has an eigenvalue ε with eigenvector $f \neq 0$, then $\Psi = a^*(f \oplus 0)a^*(0 \oplus \overline{f})\Omega_\omega \neq 0$,

$$\mathrm{e}^{\mathrm{i}tL}\Psi = a^*(\mathrm{e}^{\mathrm{i}tH}f \oplus 0)a^*(0 \oplus \mathrm{e}^{-\mathrm{i}t\overline{H}}\overline{f})\Omega_\omega = \mathrm{e}^{\mathrm{i}t(\varepsilon-\varepsilon)}a^*(f \oplus 0)a^*(0 \oplus \overline{f})\Omega_\omega = \Psi,$$

and hence $L\Psi = 0$ so that 0 is not a simple eigenvalue of L. If on the contrary H has no eigenvalues, so does $\widehat{H} = H \oplus 0 - 0 \oplus \overline{H}$. In particular, if H has purely absolutely continuous spectrum, then the spectrum of L consists of a simple eigenvalue 0 with eigenvector Ω_ω and the purely absolutely continuous spectrum

$$\left\{ \sum_{\varepsilon \in \mathrm{Sp}(H) \cup \mathrm{Sp}(-H)} n_\varepsilon \varepsilon \,\middle|\, n_\varepsilon \in \{0,1\}, \sum_{\varepsilon \in \mathrm{Sp}(H) \cup \mathrm{Sp}(-H)} n_\varepsilon < \infty \right\}^{\mathrm{cl}}.$$

However, if H has some singular spectrum, so does L_ω. Thus, the following proposition is a direct consequence of Proposition 2.10.

Proposition 3.4 *Let T be the generator of a gauge invariant quasi-free state on* $\mathrm{CAR}(\mathfrak{h})$ *such that* $\mathrm{Ker}\,(T) = \mathrm{Ker}\,(I - T) = \{0\}$ *(so that ω_T is modular). Then ω_T is ergodic if and only if H has no eigenvalue. If in addition H has empty singular continuous spectrum then ω_T is mixing.*

3.2.5 Gauge group and chemical potentials

In this section, we generalize the previous result to more general Abelian gauge groups. Suppose that there exists a family of self-adjoint operators $\{Q^{(1)}, \ldots, Q^{(N)}\}$ on $\mathfrak{h}$ such that

$$[\mathrm{e}^{\mathrm{i}tQ^{(j)}}, \mathrm{e}^{\mathrm{i}sQ^{(k)}}] = 0, \qquad [\mathrm{e}^{\mathrm{i}tH}, \mathrm{e}^{\mathrm{i}sQ^{(k)}}] = 0,$$

for all $s, t \in \mathbb{R}$ and all $j, k \in \{1, \ldots, N\}$. These operators may be interpreted as the generators of a symmetry group of the system. In fact

$$\mathbb{R}^N \ni s = (s_1, \ldots, s_N) \mapsto U(s) = \mathrm{e}^{\mathrm{i}\sum_{j=1}^N s_j Q^{(j)}} = \prod_{j=1}^N \mathrm{e}^{\mathrm{i}s_j Q^{(j)}},$$

is a strongly continuous, faithful, unitary representation of the Abelian group $G \equiv \mathbb{R}^N / K$ in $\mathfrak{h}$, where

$$K \equiv \{s \in \mathbb{R}^N \,|\, U(s) = I\},$$

is a subgroup of $\mathbb{R}^N$. We will always assume that G is compact. Since $U(s)HU^*(s) = H$, for all $s \in \mathbb{R}^N$, the Bogoliubov group $\vartheta^s(A) = \Gamma(U(s))A\Gamma(U(s))^*$ commutes with the dynamics τ_H^t. Thus, the C^*-subalgebra

$$\mathrm{CAR}_G(\mathfrak{h}) \equiv \{A \in \mathrm{CAR}(\mathfrak{h}) \,|\, \vartheta^s(A) = A \text{ for all } s \in \mathbb{R}^N\},$$

is invariant under τ_H. As a general rule, only the elements of this subalgebra are physically observable. In the presence of a gauge group G the C^*-dynamical system corresponding to our system is thus $(\mathrm{CAR}_G(\mathfrak{h}), \tau_H)$. Since ϑ acts trivially on $\mathrm{CAR}_G(\mathfrak{h})$, it is clear that for all $\mu = (\mu_1, \ldots, \mu_n) \in \mathbb{R}^N$ the unique β-KMS state on $\mathrm{CAR}(\mathfrak{h})$ for the group $t \mapsto \tau_H^t \circ \vartheta^{-t\mu}$ is a β-KMS state for the restriction of τ to $\mathrm{CAR}_G(\mathfrak{h})$. Conversely, every extremal $\langle \tau_H^t, \beta\rangle$-KMS state on $\mathrm{CAR}_G(\mathfrak{h})$ is the restriction to this subalgebra of the $\langle \tau_H^t \circ \vartheta^{-t\mu}, \beta\rangle$-KMS state on $\mathrm{CAR}(\mathfrak{h})$ for some $\mu = (\mu_1, \ldots, \mu_n) \in \mathbb{R}^N$. This state is quasi-free, generated by

$$T_{\beta,\mu} \equiv \left(1 + \mathrm{e}^{\beta(H - \sum_{j=1}^N \mu_j Q^{(j)})}\right)^{-1}.$$

We call the operators $Q^{(1)}, \ldots, Q^{(N)}$ charges. The parameters $\mu_1, \ldots, \mu_N$ are the chemical potentials associated with these charges.

Example 3.1 The following example is typical and provides an illustration of the previous discussion. Suppose that the fermions in our system are of two distinct types (and thus distinguishable), say red and blue. In this case, the one-particle Hilbert space can be written in the form $\mathfrak{h} = \mathfrak{h}_r \oplus \mathfrak{h}_b$ where $\mathfrak{h}_r$ and $\mathfrak{h}_b$ are two copies of the same space, one for the red fermions and the other for the blue ones. The wave function $f \oplus 0$ describe a red fermion while $0 \oplus f$ describes a blue fermion in the same state. In this case the charges are identified with the colors

$$Q^{(r)} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad Q^{(b)} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

and the gauge group is the two-dimensional torus $G = S^1 \times S^1$. Gauge invariance expresses the fact that the phase of each component of the wave function $f \oplus g$ is not measurable, i.e., $\psi = f \oplus g$ and $\mathrm{e}^{\mathrm{i}(s_r Q^{(r)} + s_b Q^{(b)})}\psi = \mathrm{e}^{\mathrm{i}s_r} f \oplus \mathrm{e}^{\mathrm{i}s_b} g$ describe the same state. The C^*-algebra $\mathcal{O} = \mathrm{CAR}(\mathfrak{h})$ is generated by the operators $r(f) = a(f \oplus 0)$ and $b(f) = a(0 \oplus f)$ and their adjoints $r^*(f)$ (which creates a red fermion in the state f) and $b^*(f)$ (which creates a blue fermion in the same state). The action of the gauge group G on $\mathcal{O}$ is given by the $*$-automorphisms ϑ^s, $s = (s_r, s_b) \in \mathbb{R}^2$ such that $\vartheta^s(r(f)) = \mathrm{e}^{-\mathrm{i}s_r} r(f)$, $\vartheta^s(b(f)) = \mathrm{e}^{-\mathrm{i}s_b} b(f)$. A monomial in the operators $r^\#$ and $b^\#$ is thus invariant under ϑ if it contains the same number of r and r^* factors, as well as the same number of b and b^* factors. The subalgebra $\mathcal{O}_G$ is generated by the operators $r^*(f)r(g)$, $b^*(f)b(g)$ and I. We denote by $\mathcal{O}_r$ the subalgebra generated by the operators $r^*(f)r(g)$ and I, and we denote by $\mathcal{O}_b$ the subalgebra generated by the operators $b^*(f)b(g)$ and I. It follows from the fact that $\{r(g), b^*(f')\} = (f \oplus 0, 0 \oplus f') = 0$ and $\{b(g'), r^*(f)\} = (0 \oplus g', f \oplus 0) = 0$ that we have

$$\begin{aligned}[r^*(f)r(g), b^*(f')b(g')] &= r^*(f)r(g)b^*(f')b(g') - b^*(f')b(g')r^*(f)r(g)\\ &= -r^*(f)b^*(f')r(g)b(g') + b^*(f')r^*(f)b(g')r(g)\\ &= -b^*(f')r^*(f)b(g')r(g) + b^*(f')r^*(f)b(g')r(g)\\ &= 0.\end{aligned}$$

We conclude that the elements of $\mathscr{O}_r$ commute with the elements of $\mathscr{O}_b$, which reflects the fact that the red fermions are distinguishable from the blue fermions. Since $\mathscr{O}_G$ is clearly generated by $\mathscr{O}_r$ and $\mathscr{O}_b$ we deduce that $\mathscr{O}_G = \mathscr{O}_r \otimes \mathscr{O}_b$.

If $H = H_r \oplus H_b$ is the one-particle Hamiltonian, the dynamics on $\mathscr{O}$ is given by $\tau^t(r(f)) = r(\mathrm{e}^{\mathrm{i}tH_r} f)$ and $\tau^t(b(f)) = b(\mathrm{e}^{\mathrm{i}tH_b} f)$ and commutes with the gauge group ϑ. The extremal $\langle\tau,\beta\rangle$-KMS states on $\mathscr{O}_G$ are quasi-free generated by

$$T_{\beta,\mu_r,\mu_b} = \left(1 + \mathrm{e}^{\beta(H-\mu_r Q^{(r)} - \mu_b Q^{(b)})}\right)^{-1}.$$

3.2.6 Thermodynamic limit

In Section 2.2.5 we identified the thermal equilibrium states of a C^*-dynamical system with the KMS states associated with this system. In Section 3.2.3 we introduced the chemical potential associated with a gauge symmetry group of the dynamical system. In this section, we discuss the relationship between equilibrium states and the grand canonical ensemble often used in equilibrium statistical mechanics.

Suppose we are given a net a closed subspaces $(\mathfrak{h}_v)_{v\in V}$ of the one-particle Hilbert $\mathfrak{h}$, as well as a corresponding family of self-adjoint operators H_v on $\mathfrak{h}_v$. In the usual presentation of the thermodynamic limit in statistical mechanics,

(i) $\mathfrak{h}$ is the Hilbert space of a fermion in infinite volume, for example $\mathfrak{h} = L^2(\mathbb{R}^3)$.

(ii) H is its Hamiltonian. For example $H = -\Delta$, the Laplacian on $\mathbb{R}^3$.

(iii) V is a directed family of finite boxes. For example, the cubes

$$v = v(L) \equiv \{(x_1, x_2, x_3) \in \mathbb{R}^3 \,|\, -L \le x_i \le L,\ i = 1,2,3\},$$

with $L > 0$.

(iv) $\mathfrak{h}_v$ is the Hilbert space of a fermion confined to the box v. For example,

$$\mathfrak{h}_v = \{u \in L^2(\mathbb{R}^3) \,|\, \mathrm{supp}\, u \subset v\},$$

which we will identify with $L^2(v)$.

(v) H_v is its Hamiltonian. For example, $H_v = -\Delta_{v,N}$, the Laplacian on the cube v with Neumann boundary conditions.

Let p_v be the orthogonal projection of $\mathfrak{h}$ onto $\mathfrak{h}_v$. We shall suppose that

(a) $\mathrm{s}-\lim_{v} p_v = I$.

(b) $\lim_v (H_v - z)^{-1} f = (H-z)^{-1} f$ for all $z \in \mathbb{C}\setminus\mathbb{R}$ and $f \in \cup_{v\in V}\mathfrak{h}_v$.

(c) $\mathrm{e}^{-\beta H_v} \in \mathscr{L}^1(\mathfrak{h}_v)$ for all $v \in V$ and $\beta > 0$.

We set $\mathscr{A}_v = \mathrm{CAR}(\mathfrak{h}_v)$ for all $v \in V$ and

$$\mathscr{A}_{\mathrm{loc}} \equiv \bigcup_{v\in V} \mathscr{A}_v.$$

The injections $\mathfrak{h}_v \subset \mathfrak{h}_{v'} \subset \mathfrak{h}$ naturally induce the injections $\Gamma^-(\mathfrak{h}_v) \subset \Gamma^-(\mathfrak{h}_{v'}) \subset \Gamma^-(\mathfrak{h})$ and $\mathscr{A}_v \subset \mathscr{A}_{v'} \subset \mathscr{A}$ for $v \le v'$. We thus have that $\mathscr{A}_{\mathrm{loc}} \subset \mathscr{A}$ and the condition (a) implies that $\mathscr{A}_{\mathrm{loc}}$ is dense in $\mathscr{A}$.

Condition (c) implies that the spectrum of H_v is pure point, of finite multiplicity, bounded from below and can only accumulate at $+\infty$. For $\Lambda > 0$, we define $\mathfrak{h}_{v\Lambda} \equiv F(H_v < \Lambda)\mathfrak{h}_v$, $\mathscr{A}_{v\Lambda} \equiv \mathrm{CAR}(\mathfrak{h}_{v\Lambda})$ and $P_{v\Lambda} \equiv \Gamma(F(H_v < \Lambda))$ the orthogonal projection of $\Gamma^-(\mathfrak{h}_v)$ onto the subspace $\Gamma^-(\mathfrak{h}_{v\Lambda})$. We note that $\mathfrak{h}_{v\Lambda}$, $\Gamma^-(\mathfrak{h}_{v\Lambda})$ and $\mathscr{A}_{v\Lambda}$ are all of finite dimension. Furthermore $\cup_{\Lambda>0}\mathfrak{h}_{v\Lambda}$, being dense in $\mathfrak{h}_v$, $\cup_{\Lambda>0}\mathscr{A}_{v\Lambda}$ is also dense in $\mathscr{A}_v$ and $\mathrm{s}-\lim_{\Lambda\to\infty} P_{v\Lambda} = P_v = \Gamma(p_v)$.

If we denote $\mathscr{K}_{\mu,v} \equiv \mathrm{d}\Gamma(H_v - \mu I)$ then $\mathrm{e}^{-\beta\mathscr{K}_{\mu,v}}$ is trace class,

$$\mathrm{e}^{-\beta\mathscr{K}_{\mu,v}} - \mathrm{e}^{-\beta\mathscr{K}_{\mu,v}} P_{v\Lambda} = \mathrm{e}^{-\beta\mathscr{K}_{\mu,v}}(I - P_{v\Lambda}),$$

and we deduce that

$$\lim_{\Lambda\to\infty} \mathrm{e}^{-\beta\mathscr{K}_{\mu,v}} P_{v\Lambda} = \mathrm{e}^{-\beta\mathscr{K}_{\mu,v}},$$

in the norm of $\mathscr{L}^1(\Gamma^-(\mathfrak{h}_v))$.

The grand canonical ensemble in the box v, at inverse temperature β with chemical potential μ, given by $\omega_{\beta,\mu,v}(A) = \mathrm{tr}(\rho_{\beta,\mu,v} A)$ where

$$\rho_{\beta,\mu,v} = \frac{\mathrm{e}^{-\beta\mathscr{K}_{\mu,v}}}{\mathrm{tr}_{\Gamma_-(\mathfrak{h}_v)}(\mathrm{e}^{-\beta\mathscr{K}_{\mu,v}})},$$

defines a state on $\mathscr{A}_v$. For all $A \in \cup_{\Lambda>0}\mathscr{A}_{v,\Lambda}$ we have

$$\omega_{\beta,\mu,v}(A) = \lim_{\Lambda\to\infty} \omega_{\beta,\mu,v,\Lambda}(A),$$

where

$$\omega_{\beta,\mu,v,\Lambda}(A) = \frac{\mathrm{tr}_{\Gamma^-(\mathfrak{h}_{v\Lambda})}(\mathrm{e}^{-\beta\mathscr{K}_{\mu,v}} A)}{\mathrm{tr}_{\Gamma^-(\mathfrak{h}_{v\Lambda})}(\mathrm{e}^{-\beta\mathscr{K}_{\mu,v}})}.$$

The group of $*$-automorphisms $\gamma^t_{\mu,v}(A) = \mathrm{e}^{\mathrm{i}t\mathscr{K}_{\mu,v}} A \mathrm{e}^{-\mathrm{i}t\mathscr{K}_{\mu,v}}$ on $\mathscr{B}(\Gamma^-(\mathfrak{h}_v))$ leaves the C^*-algebra $\mathscr{A}_{v\Lambda}$ invariant. Example 1 from Section 2.2.5 shows that $\omega_{\beta,\mu,v,\Lambda}$ is the unique $\langle\gamma^t_{\mu,v},\beta\rangle$-KMS state on $\mathscr{A}_{v\Lambda}$. Theorem 3.2 implies that $\omega_{\beta,\mu,v,\Lambda}$ is gauge invariant quasi-free generated by

$$T_{\beta,\mu,v,\Lambda} = (I + \mathrm{e}^{\beta(H_v - \mu I)})^{-1}|_{\mathfrak{h}_{v\Lambda}}.$$

For all $f_1,\ldots,g_1,\ldots \in \mathfrak{h}_{v\Lambda}$, we thus have

$$\begin{aligned}\omega_{\beta,\mu,v}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)) &= \lim_{\Lambda'\to\infty} \omega_{\beta,\mu,v,\Lambda'}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n))\\ &= \lim_{\Lambda'\to\infty} \delta_{nm}\det[(f_i, T_{\beta,\mu,v,\Lambda'}g_j)]_{i,j=1,\ldots n}.\end{aligned}$$

We deduce that

$$\omega_{\beta,\mu,v}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)) = \delta_{nm}\det[(f_i, T_{\beta,\mu,v}g_j)]_{i,j=1,\ldots n}.$$

where

$$T_{\beta,\mu,v} = (I + \mathrm{e}^{\beta(H_v - \mu)})^{-1}.$$

This last formula extends continuously to all $f_1,\ldots,g_1,\ldots \in \mathfrak{h}_v$. $\omega_{\beta,\mu,v}$ is thus the gauge invariant quasi-free state generated by $T_{\beta,\mu,v}$. Condition (b) implies that

$$\lim_{v'} T_{\beta,\mu,v'}f = T_{\beta,\mu}f \equiv (I + \mathrm{e}^{\beta(H-\mu)})^{-1}f,$$

for all $f \in \mathfrak{h}_v$. We deduce that

$$\begin{aligned}\omega_{\beta,\mu}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)) &\equiv \lim_{v'} \omega_{\beta,\mu,v'}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n))\\ &= \lim_{v'} \delta_{nm}\det\{(f_i, T_{\beta,\mu,v'}g_j)\}_{i,j=1,\ldots n}\\ &= \delta_{nm}\det\{(f_i, T_{\beta,\mu}g_j)\}_{i,j=1,\ldots n},\end{aligned}$$

for all $f_1,\ldots,g_1,\ldots \in \mathfrak{h}_v$. This shows that $\omega_{\beta,\mu}$, the gauge invariant quasi-free state on $\mathscr{A}$ generated by $T_{\beta,\mu}$, is the thermodynamic limit of the grand canonical ensemble

$$\omega_{\beta,\mu}(A) = \lim_{v'} \omega_{\beta,\mu,v'}(A),$$

for all $A \in \mathscr{A}_{\mathrm{loc}}$.

3.3 Open quantum systems

This section is a brief introduction to the C^*-algebraic description of open quantum systems and to the nonequilibrium statistical mechanics of these systems. For a more detailed discussion, we refer the reader to [JP7, AJPP1].

3.3.1 Algebraic description

A system is called open if it interacts with some environment. A typical example of an open quantum system is an atom (or a molecule) whose charged constituents interact with the electromagnetic field. If we neglect these interactions, an atom generally allows for a series of steady states, corresponding to the eigenvalues of its Hamiltonian. Taking into account the interaction of the electrons with the electromagnetic field, only the ground state remain stable. The excited steady states turn into metastable states with a finite lifetime (see [BFS1, BFS2] for a rigorous treatment of this fundamental effect).

To model an open system, one generally considers that the system is made up of a small, confined system $\mathscr{S}$, with a finite number of classical degrees of freedom, as well as one or several reservoirs $\mathscr{R}_1,\dots,\mathscr{R}_M$, each of those being an extended system with a large number of degrees of freedom. While the small system $\mathscr{S}$ may have a complex internal structure, the reservoirs are generally simple systems, for example ideal gases. In terms of Hamiltonians, the dynamics of such a system is determined, at least formally, by the sum

$$H^{\mathrm{tot}} = H_{\mathscr{S}} + \sum_{j=1}^{M} H_{\mathscr{R}_j} + \sum_{j=1}^{M} H^{\mathrm{int}}_{\mathscr{S},\mathscr{R}_j},$$

where $H_{\mathscr{S}}$ is the Hamiltonian of the small system, $H_{\mathscr{R}_j}$ is that of reservoir $\mathscr{R}_j$, and $H^{\mathrm{int}}_{\mathscr{S},\mathscr{R}_j}$ is the Hamiltonian representing the interaction between the small system and reservoir $\mathscr{R}_j$.

In a mathematically rigorous approach to open systems it is often convenient to idealize the reservoirs and consider them to be infinitely extended (this is in particular the case for the construction of nonequilibrium steady states). In such situations the algebraic formulation of quantum dynamics provides a more appropriate framework than the familiar Hilbert space/Hamiltonian approach. The coupled system $\mathscr{S}+\mathscr{R}_1+\cdots\mathscr{R}_M$ is described by a C^*-dynamical system $\langle\mathscr{O},\tau\rangle$ which has the following structure

(i) There exist C^*-subalgebras $\mathscr{O}_{\mathscr{S}},\mathscr{O}_{\mathscr{R}_1},\dots\mathscr{O}_{\mathscr{R}_{\mathrm{M}}}\subset\mathscr{O}$, such that $\mathscr{O}_{\mathscr{S}}\cap\mathscr{O}_{\mathscr{R}_j}=\mathscr{O}_{\mathscr{R}_k}\cap\mathscr{O}_{\mathscr{R}_j}=\mathbb{C}I$ for $j\neq k$ and

$$\mathscr{O}=\mathscr{O}_{\mathscr{S}}\vee\mathscr{O}_{\mathscr{R}_1}\vee\cdots\vee\mathscr{O}_{\mathscr{R}_{\mathrm{M}}},$$

that is to say that $\mathscr{O}$ is generated by these subalgebras. $\mathscr{O}_{\mathscr{S}}$ is the algebra of observables of the small system, and $\mathscr{O}_{\mathscr{R}_j}$ is that of the j-th reservoir.

(ii) For each $\alpha\in\{\mathscr{S},\mathscr{R}_1,\dots,\mathscr{R}_M\}$ there exists a C^*-dynamical system $\langle\mathscr{O},\tau_\alpha\rangle$ such that $\tau_\alpha^t(\mathscr{O}_\alpha)\subset\mathscr{O}_\alpha$ and $\tau_\alpha^t(A)=A$ for $A\in\mathscr{O}_\beta$ and $\beta\neq\alpha$. The C^*-dynamical systems $\langle\mathscr{O}_\alpha,\tau_\alpha|_{\mathscr{O}_\alpha}\rangle$ describe the components of the system without interactions between them.

(iii) $\tau^t_{\mathscr{S}}=\mathrm{e}^{t\delta_{\mathscr{S}}}$ where the $*$-derivation $\delta_{\mathscr{S}}$ is inner, i.e., there exists a self-adjoint element $H_{\mathscr{S}}\in\mathscr{O}_{\mathscr{S}}$ such that $\delta_{\mathscr{S}}=\mathrm{i}[H_{\mathscr{S}},\cdot]$.

(iv) Let $\delta, \delta_{\mathscr{R}_j}$ be the $*$-derivations generating the C^*-dynamics $\tau, \tau_{\mathscr{R}_j}$. There exist self-adjoint elements $V_j \in \mathscr{O}_{\mathscr{S}} \vee \mathscr{O}_{\mathscr{R}_j}$ such that

$$\delta(A) = \delta_{\mathscr{S}}(A) + \sum_{j=1}^{M} \delta_{\mathscr{R}_j}(A) + \sum_{j=1}^{M} \mathrm{i}[V_j, A].$$

V_j thus describes the interaction between the small system and the j-th reservoir.

The dynamics of the system admits a perturbative expansion, the Schwinger-Dyson series

$$\tau^t(A) = \tau_0^t(A) + \sum_{n=1}^{\infty} \int_{0 \le s_1 \le \cdots \le s_n \le t} \mathrm{i}[\tau_0^{s_1}(V), \mathrm{i}[\cdots, \mathrm{i}[\tau_0^{s_n}(V), \tau_0^t(A)]\cdots]]\, \mathrm{d}s_1 \cdots \mathrm{d}s_n,$$

where $\tau_0^t = \mathrm{e}^{t\delta_0}$ with $\delta_0 = \delta_{\mathscr{S}} + \sum_{j=1}^{M} \delta_{\mathscr{R}_j}$ and $V = \sum_{j=1}^{M} V_j$. This series converges in the norm of $\mathscr{O}$ for all $t \in \mathbb{R}$ and $A \in \mathscr{O}$.

3.3.2 Non-equilibrium steady states (NESS)

Let $\omega \in E(\mathscr{O})$ be the initial state of the system. If this state is close enough to a thermodynamic equilibrium ω_{eq} it is expected that the system will relax towards equilibrium,

$$\lim_{t\to\infty} \omega \circ \tau^t(A) = \omega_{\mathrm{eq}}(A),$$

for all $A \in \mathscr{O}$. On the other hand, if ω is sufficiently far from a thermodynamic equilibrium state, the system may evolve to a nonequilibrium steady state.

Following Ruelle ([R2, R3]) we define a nonequilibrium steady state (NESS) associated with the initial state ω as a limit point, in the weak-$*$ topology of $E(\mathscr{O}) \subset \mathscr{O}'$, of the net

$$\langle\omega\rangle_t \equiv \frac{1}{t}\int_0^t \omega \circ \tau^s ds,$$

with $t > 0$. We denote by $\Sigma^+(\omega)$ the set of all NESS associated to ω. We thus have $\omega^+ \in \Sigma^+(\omega)$ if and only if there exists a net $t_\alpha \to +\infty$ such that

$$\lim_{\alpha} \langle\omega\rangle_{t_\alpha}(A) = \omega^+(A), \tag{29}$$

for all $A \in \mathscr{O}$. One can easily show that all elements of $\Sigma^+(\omega)$ are τ-invariant states. Furthermore, since $E(\mathscr{O})$ is weak-$*$ compact, $\Sigma^+(\omega)$ is never empty. The fundamental problem of nonequilibrium statistical mechanics of the system $\langle\mathscr{O}, \tau\rangle$ is the study of the properties of these NESS. We are particularly interested in showing that $\Sigma^+(\omega) = \{\omega^+\}$ (there is only one NESS), and that

$$\lim_{t\to\infty} \omega \circ \tau^t(A) = \omega^+(A), \tag{30}$$

the unique NESS, is an attractor.

3.3.3 Scattering theory of C^*-dynamical systems

As already remarked in the introduction, three methods have been implemented to study the limit in equation (30):

- Ruelle's scattering approach [R4] uses scattering theory of C^*-dynamical systems to construct a unique NESS. This method operates directly on the algebra $\mathcal{O}$ without passing to a representation.
- The spectral method of Jakšić-Pillet [JP6] (see also [MMS]). It reduces the problem to the analysis of the complex resonances of a Liouvillean, a non self-adjoint generator of the dynamics in the canonical cyclic representation of the C^*-algebra $\mathcal{O}$ associated with the initial state ω.
- The de Roeck-Kupiainen cluster expansion technique [dRK1, dRK2] which operates directly on the sample subalgebra $\mathcal{O}_{\mathcal{S}}$.

We shall apply the first approach in these notes. In the following, we provide a general description of this method. We refer the reader to [R4, R5, JP7, AJPP1] for further discussion and to [DFG, FMU, FMSU, JOP1, JPP2, CMP1, CMP2] for examples of application of the method.

The C^*-algebraic scattering theory is inspired by the Hilbert space scattering theory introduced in Section 2.1.4 and relies on the existence of the strong limits

$$\gamma^{\pm} = \mathrm{s}-\lim_{t\to\pm\infty} \tau_0^{-t}\circ\tau^t, \tag{31}$$

(compare with Eq. (11), and observe that the order of the free and perturbed groups is reversed since we are working here in the Heisenberg picture whereas the Hilbert space scattering is formulated in the Schrödinger picture). The groups τ_0 and τ being isometric, these limits, if they exist, define injective $*$-endomorphisms of $\mathcal{O}$ such that

$$\gamma^{\pm}\circ\tau^t = \tau_0^t\circ\gamma^{\pm},$$

for all $t\in\mathbb{R}$. We call them Møller morphisms. As in the Hilbert spaces theory, the τ_0-invariant C^*-subalgebras $\mathcal{O}^{\pm}\equiv\gamma^{\pm}(\mathcal{O})$ play a central role. For all $A\in\mathcal{O}$, we have

$$0 = \lim_{t\to\pm\infty}\|\gamma^{\pm}(A) - \tau_0^{-t}\circ\tau^t(A)\| = \lim_{t\to\pm\infty}\|\tau_0^t(\gamma^{\pm}(A)) - \tau^t(A)\|,$$

that is to say that the evolution of A under τ is asymptotically that of $\gamma^{\pm}(A)$ under τ_0 when $t\to\pm\infty$. We may thus define a $*$-isomorphism

$$\sigma\equiv\gamma^{+}\circ(\gamma^{-})^{-1}:\mathcal{O}^{-}\to\mathcal{O}^{+},$$

which transforms the incoming asymptote $\gamma^{-}(A)$ into the outgoing asymptote $\gamma^{+}(A)$. It is evidently the equivalent to the scattering operator in the Hilbert space approach.

For all $A \in \mathcal{O}$ one has

$$0 = \lim_{t \to \pm\infty} \|\tau_0^t(\gamma^\pm(A)) - \tau^t(A)\| = \lim_{t \to \pm\infty} \|\tau^{-t} \circ \tau_0^t(\gamma^\pm(A)) - A\|,$$

which shows that the strong limits

$$\alpha^\pm = \mathrm{s}-\lim_{t \to \pm\infty} \tau^{-t} \circ \tau_0^t|_{\mathcal{O}^\pm}, \tag{32}$$

exists and that $\alpha^\pm = (\gamma^\pm)^{-1}$.

In the context of open systems described in the preceding section we expect

$$\mathcal{O}^- = \mathcal{O}^+ = \mathcal{O}_{\mathcal{R}} \equiv \bigvee_{j=1}^{M} \mathcal{O}_{\mathcal{R}_j}, \tag{33}$$

where $\mathcal{O}_{\mathcal{R}}$ is the C^*-subalgebra of the reservoirs. In fact, the small system $\mathcal{S}$ being confined, the spectrum of its Hamiltonian $H_{\mathcal{S}}$ will be pure point. In this case $\delta_{\mathcal{S}} = \mathrm{i}[H_{\mathcal{S}}, \cdot]$ will also have a pure point spectrum and we thus do not expect that the limit in Eq. (32) exists on $\mathcal{O}_{\mathcal{S}}$.

We note in particular that if (33) is verified then $\gamma^\pm$ provide $*$-isomorphisms between the C^*-dynamical systems $\langle \mathcal{O}, \tau \rangle$ and $\langle \mathcal{O}_{\mathcal{R}}, \tau_{\mathcal{R}} \rangle$ where $\tau_{\mathcal{R}} = \tau_0|_{\mathcal{O}_R}$ denotes the free dynamics of the reservoirs. If the initial state ω is τ_0-invariant, then

$$\omega \circ \tau^t = \omega \circ \tau_0^{-t} \circ \tau^t,$$

and

$$\lim_{t \to \pm\infty} \omega \circ \tau^t(A) = \lim_{t \to \pm\infty} \omega \circ \tau_0^{-t} \circ \tau^t(A) = \omega|_{\mathcal{O}_{\mathcal{R}}} \circ \gamma^\pm(A),$$

for all $A \in \mathcal{O}$. From this we get that $\Sigma^+(\omega) = \{\omega^+\}$ and the unique NESS associated with ω is independent of the initial state of the small system $\omega|_{\mathcal{O}_{\mathcal{S}}}$. If $\omega|_{\mathcal{O}_{\mathcal{R}}}$ has ergodic properties (which is typically the case for ideal reservoirs) we can say even more. For all $\nu \in E(\mathcal{O})$, we have

$$|\nu \circ \tau^t(A) - \nu \circ \tau_0^t(\gamma^+(A))| \le \|\tau^t(A) - \tau_0^t(\gamma^+(A))\| = \|\tau_0^{-t} \circ \tau^t(A) - \gamma^+(A)\|,$$

and thus

$$\lim_{t \to \infty} |\nu \circ \tau^t(A) - \nu \circ \tau_0^t(\gamma^+(A))| = 0.$$

If $\omega|_{\mathcal{O}_{\mathcal{R}}}$ is $\tau_{\mathcal{R}}$-ergodic and if $\nu|_{\mathcal{O}_{\mathcal{R}}}$ is $\omega|_{\mathcal{O}_{\mathcal{R}}}$-normal, we deduce that

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \nu \circ \tau^t(A)\, \mathrm{d}t = \lim_{T \to \infty} \frac{1}{T} \int_0^T \nu \circ \tau_0^t(\gamma^+(A))\, \mathrm{d}t = \omega(\gamma^+(A)),$$

that is to say $\Sigma^+(\nu) = \{\omega^+\}$. Similarly, if $\omega|_{\mathcal{O}_{\mathcal{R}}}$ is $\tau_{\mathcal{R}}$-mixing and if $\nu|_{\mathcal{O}_{\mathcal{R}}}$ is $\omega|_{\mathcal{O}_{\mathcal{R}}}$-normal,

$$\lim_{t \to \infty} \nu \circ \tau^t(A) = \lim_{t \to \infty} \nu \circ \tau_0^t(\gamma^+(A)) = \omega(\gamma^+(A)).$$

Ruelle's approach may thus be summarized by the following proposition

Proposition 3.5 *Suppose that the Møller morphism γ^+ defined in Eq. (31) exists and is such that $\gamma^+(\mathscr{O}) = \mathscr{O}_{\mathscr{R}}$. If ω is τ_0-invariant, then, for all $A \in \mathscr{O}$,*

$$\lim_{t\to\infty} \omega \circ \tau^t(A) = \omega^+(A),$$

where $\omega^+ = \omega|_{\mathscr{O}_{\mathscr{R}}} \circ \gamma^+$. In particular, we have $\Sigma^+(\omega) = \{\omega^+\}$ and the unique NESS ω^+ associated with ω is independent of the initial state of the small system $\mathscr{S}$. If $\omega|_{\mathscr{O}_{\mathscr{R}}}$ is $\tau_{\mathscr{R}}$-ergodic, we have $\Sigma^+(\nu) = \{\omega^+\}$ for all $\nu \in E(\mathscr{O})$ such that $\nu|_{\mathscr{O}_{\mathscr{R}}}$ is $\omega|_{\mathscr{O}_{\mathscr{R}}}$-normal. If, furthermore, $\omega|_{\mathscr{O}_{\mathscr{R}}}$ is $\tau_0|_{\mathscr{O}_{\mathscr{R}}}$-mixing, then

$$\lim_{t\to\infty} \nu \circ \tau^t(A) = \omega^+(A),$$

holds for all $A \in \mathscr{O}$ and all $\nu \in E(\mathscr{O})$ such that $\nu|_{\mathscr{O}_{\mathscr{R}}}$ is $\omega|_{\mathscr{O}_{\mathscr{R}}}$-normal.

3.3.4 Entropy production

Another central notion in nonequilibrium statistical mechanics is entropy production. The general definition of entropy production is problematic since the concept of entropy itself – fundamental for equilibrium thermodynamics – does not have a satisfying generalization outside of equilibrium (the reader interested in this problematic should read the following enlightening discussions by Gallavotti and Ruelle [G1, G2, R5, R6, R7, R8]).

Following Ruelle [R5] and Jakšić-Pillet [P1, JP5, JP4] we can however give a satisfactory definition of entropy production for a large class of NESS. This definition is based on the concept of relative entropy (we refer to [O, OHI, LS, Sp3] for similar considerations and to [AF2] for a careful analysis of entropy production in the framework of cyclic processes).

The relative entropy of two density matrices ρ and ω on a Hilbert space $\mathscr{H}$ is defined, analogously to the relative entropy of two measures, by the formula

$$\mathrm{Ent}(\rho|\omega) \equiv \mathrm{tr}(\rho(\log\omega - \log\rho)).$$

Let $(\varphi_i)_i$ be an orthonormal basis of eigenvectors of ρ and let p_i be the associated eigenvalues. Then $p_i \in [0,1]$ and $\sum_i p_i = 1$. Let $q_i \equiv (\varphi_i, \omega\varphi_i)$. We thus have that $q_i \in [0,1]$ and $\sum_i q_i = \mathrm{tr}(\omega) = 1$. By applying Jensen's inequality twice we get (with the convention $0\log 0 = 0$)

$$\begin{aligned}\mathrm{Ent}(\rho|\omega) &= \sum_i p_i((\varphi_i, \log\omega\varphi_i) - \log p_i) \\ &\leq \sum_i p_i(\log q_i - \log p_i) \leq \log\sum_i q_i = 0.\end{aligned}$$

We thus have that $\mathrm{Ent}(\rho|\omega) \leq 0$. We can also show that $\mathrm{Ent}(\rho|\omega) = 0$ if and only if $\rho = \omega$. Araki extended this definition to states of a C^*-algebra [A1, A2] (see also [OP, BR2]). We will not go into the details of this extension, which is based on the modular theory of Tomita and Takesaki. The only property of this extension of interest to us is precisely the one which we describe in the following result ([JP5]).

Theorem 3.6 *Let $\omega \in E(\mathcal{O})$ be a τ_0-invariant state. Suppose that ω is $\langle\sigma_\omega, 1\rangle$-KMS for a group $t \mapsto \sigma_\omega^t$ of $*$-automorphisms of $\mathcal{O}$. We denote by δ_ω the $*$-derivation generating the group σ_ω. If $V \in \mathrm{Dom}(\delta_\omega)$ then*

$$\mathrm{Ent}(\nu \circ \tau^t | \omega) = \mathrm{Ent}(\nu|\omega) + \int_0^t \nu \circ \tau^s(\delta_\omega(V))\,\mathrm{d}s,$$

for all $\nu \in E(\mathcal{O})$.

We shall use this result to define the entropy production rate of a NESS. In order to get a convincing physical interpretation of this definition we will restrict ourselves to initial states ω which are close enough to "product states" in which each reservoir is in thermal equilibrium. Let $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_M) \in \mathbb{R}_+^M$. We say that $\omega_{\boldsymbol{\beta}}$ is a $\boldsymbol{\beta}$-KMS state if it is a $\langle\sigma_{\boldsymbol{\beta}}, 1\rangle$-KMS state, where $\sigma_{\boldsymbol{\beta}}$ denotes the group of $*$-automorphisms of $\mathcal{O}$ generated by

$$\delta_{\boldsymbol{\beta}} = \sum_{j=1}^M \beta_j \delta_{\mathcal{R}_j}.$$

To simplify our exposition we shall always assume here that such a state exists and is unique (this is the case if the reservoirs are ideal Fermi gases, which is the situation that will prevail in the remaining parts of these notes). Remark 3 of Section 2.2.5 shows that the restricted state $\omega_{\boldsymbol{\beta}}|_{\mathcal{O}_{\mathcal{R}_j}}$ is a β_j-KMS state for $\tau_{\mathcal{R}_j}$, i.e., in the state $\omega_{\boldsymbol{\beta}}$ each reservoir is in thermal equilibrium. However, if the β_j are not all equal then the joint reservoir system $\mathcal{R}$ is not in a global equilibrium state.

Applying the results of Section 2.2.6, for any self-adjoint $K \in \mathcal{O}$

$$\delta_{\boldsymbol{\beta}}^{(K)} = \delta_{\boldsymbol{\beta}} + \mathrm{i}[K, \cdot],$$

generates a dynamics $\sigma_{\boldsymbol{\beta}}^{(K)}$ with a unique $\langle\sigma_{\boldsymbol{\beta}}^{(K)}, 1\rangle$-KMS state $\omega_{\boldsymbol{\beta}}^{(K)} \in E(\mathcal{O})$. The set $E_{\boldsymbol{\beta}}(\mathcal{O})$ of all states obtained in this way is dense in the set $\mathcal{N}_{\omega_{\boldsymbol{\beta}}}$ of all $\omega_{\boldsymbol{\beta}}$-normal states. Moreover, one has the estimates [A3, A4]

$$\omega_{\boldsymbol{\beta}}^{(K)}(K) - \omega_{\boldsymbol{\beta}}(K) \le \mathrm{Ent}(\omega_{\boldsymbol{\beta}}^{(K)}|\omega_{\boldsymbol{\beta}}) \le \omega_{\boldsymbol{\beta}}^{(K)}(K) + \log \omega_{\boldsymbol{\beta}}(\mathrm{e}^{-K}). \tag{34}$$

Let $\omega \in E_{\boldsymbol{\beta}}(\mathcal{O})$ and $\omega^+ \in \Sigma^+(\omega)$ so that Eq. (29) holds for a net t_α. We define the entropy production rate of ω^+ by

$$\mathrm{Ep}(\omega^+) = -\lim_\alpha \frac{1}{t_\alpha} \mathrm{Ent}(\omega \circ \tau^{t_\alpha}|\omega_{\boldsymbol{\beta}}). \tag{35}$$

Assuming that $V_j \in \mathrm{Dom}(\delta_{\mathcal{R}_j})$ for all j, Theorem 3.6 allows us to write

$$\frac{1}{t_\alpha}\mathrm{Ent}(\omega \circ \tau^{t_\alpha}|\omega_{\boldsymbol{\beta}}) = \frac{1}{t_\alpha}\mathrm{Ent}(\omega|\omega_{\boldsymbol{\beta}}) + \frac{1}{t_\alpha}\int_0^{t_\alpha} \omega \circ \tau^s(\delta_{\boldsymbol{\beta}}(V))\,\mathrm{d}s,$$

and we deduce from Eq. (29) and (34) that

$$\mathrm{Ep}(\omega^+) \equiv \omega^+(-\delta_{\boldsymbol{\beta}}(V)). \tag{36}$$

We will come back to the physical interpretation of this relation in the following section. Meanwhile, we note that the inequality

$$\mathrm{Ep}(\omega^+) \geq 0,$$

is a consequence of the fact that the relative entropy of two states is never positive.

3.3.5 First and second laws of thermodynamics

To legitimate Definition (35) and interpret Relation (36) we discuss in this section the first two laws of thermodynamics in the framework of open quantum systems. To do this, we must identify the observables Φ_j which describe the energy flux leaving the reservoirs $\mathscr{R}_j$ and entering the small system $\mathscr{S}$.

As in the preceding section, we shall assume that $V_j \in \mathrm{Dom}(\delta_{\mathscr{R}_j})$ for $j = 1, \ldots, M$. The total energy flux leaving the reservoirs is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\tau^t(H_{\mathscr{S}} + V) = \tau^t(\delta(H_{\mathscr{S}} + V)).$$

Since

$$\delta(H_{\mathscr{S}} + V) = \mathrm{i}[H_{\mathscr{S}} + V, H_{\mathscr{S}} + V] + \sum_{j=1}^{M} \delta_{\mathscr{R}_j}(H_{\mathscr{S}} + V),$$

and $\delta_{\mathscr{R}_j}(H_{\mathscr{S}}) = 0$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\tau^t(H_{\mathscr{S}} + V) = \sum_{j=1}^{M} \tau^t(\delta_{\mathscr{R}_j}(V)).$$

We may thus identify

$$\Phi_j = \delta_{\mathscr{R}_j}(V) = \delta_{\mathscr{R}_j}(V_j),$$

as the observable describing the energy flux leaving the j-th reservoir. The identity

$$\sum_{j=1}^{M} \Phi_j = \delta(H_{\mathscr{S}} + V),$$

expresses the conservation of energy – the first law of thermodynamics: for any τ-invariant state ν,

$$\sum_{j=1}^{M} \nu(\Phi_j) = \frac{\mathrm{d}}{\mathrm{d}t}\nu \circ \tau^t(H_{\mathscr{S}} + V)\bigg|_{t=0} = 0.$$

Relation (36) can now be written as

$$\mathrm{Ep}(\omega^+) = -\sum_{j=1}^{M} \beta_j \omega^+(\Phi_j),$$

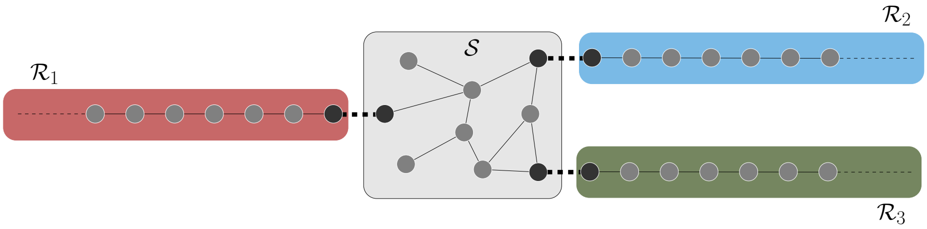

Figure 2: A discrete structure $\mathfrak{M} = \mathscr{S} \cup \mathscr{R}_1 \cup \mathscr{R}_2 \cup \mathscr{R}_3$.

which can be interpreted as an entropy balance equation. Its right hand side is the phenomenological expression of the entropy flux leaving the system $\mathscr{S}$ and must coincide with the entropy produced within this system (see for example [DGM]). In particular, for all NESS $\omega^+ \in \Sigma^+(\omega)$, we obtain

$$\sum_{j=1}^{M} \beta_j \omega^+(\Phi_j) = -\mathrm{Ep}(\omega_+) \leq 0,$$

which is an expression of the second law of thermodynamics.

3.4 Open fermionic systems

In this section, we show how to adapt the description of open systems developed in Section 3.3 to the special case of quasi-free fermionic systems. We shall see that scattering theory takes a particularly simple form in this case.

3.4.1 The one-particle setup

In order to simplify the presentation and avoid unnecessary technical difficulties we consider an ideal Fermi gas on a connected discrete structure $\mathfrak{M}$ which is the disjoint union of a finite set $\mathscr{S}$ and of M semi-infinite one-dimensional lattices $\mathscr{R}_1, \ldots, \mathscr{R}_M$ (see Figure 2). This situation is typical of the tight binding approximation widely used in solid state physics. The one-particle Hilbert space admits the following decomposition

$$\mathfrak{h} = \mathfrak{h}_{\mathscr{S}} \oplus \mathfrak{h}_{\mathscr{R}}, \qquad \mathfrak{h}_{\mathscr{R}} = \bigoplus_{k=1}^{M} \mathfrak{h}_k,$$

where $\mathfrak{h}_{\mathscr{S}} = \ell^2(\mathscr{S})$ and $\mathfrak{h}_k = \ell^2(\mathscr{R}_k)$ with $\mathscr{R}_k = \mathbb{N}$. Let $H_{\mathscr{S}}$ be a self-adjoint operator on $\mathfrak{h}_{\mathscr{S}}$ which describes the internal structure of the sample $\mathscr{S}$. For each k denote by H_k a copy of the discrete Laplacian on $\mathbb{N}$ with Dirichlet boundary condition, i.e., the operator on $\ell^2(\mathbb{N})$ defined by

$$(Lu)(x) = \frac{1}{2} \sum_{|x-y|=1} u(y).$$

It is the standard tight binding Hamiltonian for an electron in a single band of a one-dimensional lead. One easily checks that

$$(Uu)(\varepsilon) = \sqrt{\frac{2}{\pi\sqrt{1-\varepsilon^2}}} \sum_{x\in\mathbb{N}} u(x)\sin(\arccos(\varepsilon)(x+1)), \tag{37}$$

defines a unitary operator from $\ell^2(\mathbb{N})$ to $L^2([-1,1],\mathrm{d}\varepsilon)$ such that $(ULu)(\varepsilon) = \varepsilon(Uu)(\varepsilon)$. Thus, H_k has purely absolutely continuous spectrum $\mathrm{Sp}(H_k) = \mathrm{Sp}_{\mathrm{ac}}(H_k) = [-1,1]$, $\mathrm{Sp}_{\mathrm{sing}}(H_k) = \emptyset$.
The one-particle Hamiltonian is given by

$$H = (H_{\mathscr{S}} \oplus H_{\mathscr{R}}) + V, \qquad H_{\mathscr{R}} = \bigoplus_{k=1}^{M} H_k,$$

with a coupling term

$$V = \sum_{k=1}^{M} \left(\chi_k(\delta_{0_k},\cdot) + \delta_{0_k}(\chi_k,\cdot)\right),$$

where $\chi_k \in \mathfrak{h}_{\mathscr{S}}$ and $\delta_{0_k} \in \mathfrak{h}_{\mathscr{R}_k}$ denotes the Kronecker delta function at site 0. Since $H_{\mathscr{S}} + V$ is compact (in fact finite rank), it follows from Weyl's theorem that $\mathrm{Sp}_{\mathrm{ess}}(H) = \mathrm{Sp}_{\mathrm{ess}}(H_{\mathscr{R}}) = [-1,1]$. To simplify our discussion, we shall assume that H has purely absolutely continuous spectrum. In the so called fully resonant case, i.e., when $\mathrm{Sp}(H_{\mathscr{S}}) \subset]-1,1[$, this condition is verified provided the coupling strength $\max_k \|\chi_k\|$ is small enough. We will discuss the effect of singular spectra in Sections 5 and 6.

3.4.2 Quasi-free NESS

We define the C^*-algebras

$$\mathscr{O} \equiv \mathrm{CAR}(\mathfrak{h}), \quad \mathscr{O}_{\mathscr{S}} \equiv \mathrm{CAR}(\mathfrak{h}_{\mathscr{S}}), \quad \mathscr{O}_{\mathscr{R}} \equiv \mathrm{CAR}(\mathfrak{h}_{\mathscr{R}}), \quad \mathscr{O}_{\mathscr{R}_k} \equiv \mathrm{CAR}(\mathfrak{h}_k),$$

and denote by τ the C^*-dynamics on $\mathscr{O}$ associated to H, i.e., $\tau^t(a^\#(f)) = a^\#(\mathrm{e}^{\mathrm{i}tH}f)$. Let T be the generator of a gauge invariant quasi-free state $\omega_T \in E(\mathscr{O})$. For all $f_1,\ldots,g_1,\ldots \in \mathfrak{h}$ we have

$$\begin{aligned}
\omega_T \circ \tau^t(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)) &= \omega_T(a^*(\mathrm{e}^{\mathrm{i}tH}g_m)\cdots a^*(\mathrm{e}^{\mathrm{i}tH}g_1)a(\mathrm{e}^{\mathrm{i}tH}f_1)\cdots a(\mathrm{e}^{\mathrm{i}tH}f_n))\\
&= \delta_{nm}\det\{(\mathrm{e}^{\mathrm{i}tH}f_i, T\mathrm{e}^{\mathrm{i}tH}g_j)\}_{i,j=1,\ldots,n}\\
&= \delta_{nm}\det\{(f_i, T_t g_j)\}_{i,j=1,\ldots,n}\\
&= \omega_{T_t}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)),
\end{aligned}$$

where $T_t \equiv \mathrm{e}^{-\mathrm{i}tH}T\mathrm{e}^{\mathrm{i}tH}$. We conclude that

$$\omega_T \circ \tau^t = \omega_{T_t}. \tag{38}$$

Furthermore if

$$T^+ \equiv \mathrm{w}-\lim_{t\to+\infty} T_t, \tag{39}$$

exists, then

$$\lim_{t\to+\infty} \omega_T\circ\tau^t(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)) = \omega_{T^+}(a^*(g_m)\cdots a^*(g_1)a(f_1)\cdots a(f_n)).$$

The mapping $A\mapsto\omega_{T_t}(A)$, being uniformly continuous in $t\in\mathbb{R}$ and the monomials $a^*(g_m)\cdots a(f_n)$ forming a total subset of $\mathscr{O}$, we can conclude that

$$\Sigma^+(\omega_T) = \{\omega_{T^+}\}. \tag{40}$$

3.4.3 Multi-channel scattering

In the preceding subsection, we reduced the problem of the existence and uniqueness of the NESS associated with a gauge invariant quasi-free state on $\mathscr{O}$ to the existence of the weak limit (39). To control this limit we will, in this subsection, implement the theory of multi-channel scattering. We present here a simplified version. A more detailed discussion will be made in Section 5.4.

Let $\tau_{\mathscr{R}_k}$ denotes the C^*-dynamics generated by H_k on $\mathscr{O}_{\mathscr{R}_k}$. Since the canonical injections $J_k:\mathfrak{h}_k\to\mathfrak{h}$ are partial isometries, we have $J_j^*J_k=\delta_{jk}I_{\mathfrak{h}_k}$ and $J_kJ_k^*=1_k$ is the orthogonal projection of $\mathfrak{h}$ onto the subspace $\mathfrak{h}_k$.

Since $HJ_k-J_kH_k=(H_{\mathscr{S}}+V)J_k$ is trace class, it follows from Pearson's theorem (Theorem XI.7 in [RS3]) that the partial Møller operators

$$\Omega_k^\pm \equiv \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}J_k\mathrm{e}^{-\mathrm{i}tH_k}P_{\mathrm{ac}}(H_k), \tag{41}$$

exist. Like the ordinary Møller operators, they satisfy the intertwining relations $f(H)\Omega_k^\pm = \Omega_k^\pm f(H_k)$ which imply in particular that $\mathrm{Ran}\,(\Omega_k^\pm)\subset\mathfrak{h}_{\mathrm{ac}}(H)$. For any $u,v\in\mathfrak{h}$ one has

$$\begin{aligned}
(\Omega_j^\pm u,\Omega_k^\pm v) &= \lim_{t\to\pm\infty}(\mathrm{e}^{\mathrm{i}tH}J_j\mathrm{e}^{-\mathrm{i}tH_j}P_{\mathrm{ac}}(H_j)u,\mathrm{e}^{\mathrm{i}tH}J_k\mathrm{e}^{-\mathrm{i}tH_k}P_{\mathrm{ac}}(H_k)v)\\
&= \lim_{t\to\pm\infty}(J_j\mathrm{e}^{-\mathrm{i}tH_j}P_{\mathrm{ac}}(H_j)u,J_k\mathrm{e}^{-\mathrm{i}tH_k}P_{\mathrm{ac}}(H_k)v)\\
&= \lim_{t\to\pm\infty}\delta_{jk}(\mathrm{e}^{-\mathrm{i}tH_k}P_{\mathrm{ac}}(H_k)u,\mathrm{e}^{-\mathrm{i}tH_k}P_{\mathrm{ac}}(H_k)v)\\
&= \delta_{jk}(u,P_{\mathrm{ac}}(H_k)v),
\end{aligned}\tag{42}$$

from which we conclude that $\Omega_k^\pm$ is a partial isometry with initial space $\mathfrak{h}_{k,\mathrm{ac}}(H_k)$ and final space $\mathrm{Ran}\,(\Omega_k^\pm)$. Moreover, the subspaces $\mathrm{Ran}\,(\Omega_k^\pm)$ are orthogonal to each other.

Pearson's theorem also implies the existence of the strong limits

$$W_k^\pm \equiv \mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tH_k}J_k^*\mathrm{e}^{-\mathrm{i}tH}P_{\mathrm{ac}}(H). \tag{43}$$

Repeating the arguments of the previous paragraph, we obtain that $W_k^\pm$ is a partial isometry with initial space $\mathfrak{h}_{\mathrm{ac}}(H)$ and final space $\mathrm{Ran}\,(W_k^\pm)\subset\mathfrak{h}_{\mathrm{ac}}(H_k)$. Thus, one has

$$\begin{aligned}
(W_k^\pm u,v) &= \lim_{t\to\pm\infty}(\mathrm{e}^{\mathrm{i}tH_k}J_k^*\mathrm{e}^{-\mathrm{i}tH}P_{\mathrm{ac}}(H)u,P_{\mathrm{ac}}(H_k)v)\\
&= \lim_{t\to\pm\infty}(P_{\mathrm{ac}}(H)u,\mathrm{e}^{\mathrm{i}tH}J_k\mathrm{e}^{-\mathrm{i}tH_k}P_{\mathrm{ac}}(H_k)v) = (u,\Omega_k^\pm v),
\end{aligned}$$

which shows that $W_k^\pm = \Omega_k^{\pm *}$.

We note that $\sum_k J_k J_k^* = \sum_k 1_k = I - 1_{\mathscr{S}}$, where $1_{\mathscr{S}}$ denotes the orthogonal projection of $\mathfrak{h}$ onto $\mathfrak{h}_{\mathscr{S}}$. Since $\mathfrak{h}_{\mathscr{S}}$ is finite dimensional, $1_{\mathscr{S}}$ is compact and it follows from the Riemann-Lebesgue lemma, Eq. (8), that

$$\begin{aligned}
\sum_k (u, \Omega_k^\pm \Omega_k^{\pm *} v) = \sum_k (W_k^\pm u, W_k^\pm v) &= \sum_k \lim_{t\to\pm\infty} (\mathrm{e}^{\mathrm{i}tH_k} J_k^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) u, \mathrm{e}^{\mathrm{i}tH_k} J_k^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) v) \\
&= \sum_k \lim_{t\to\pm\infty} (J_k^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) u, J_k^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) v) \\
&= \sum_k \lim_{t\to\pm\infty} (\mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) u, J_k J_k^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) v) \\
&= (u, P_{\mathrm{ac}}(H) v) - \lim_{t\to\pm\infty} (\mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) u, 1_{\mathscr{S}} \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{ac}}(H) v) \\
&= (u, P_{\mathrm{ac}}(H) v).
\end{aligned}$$

Thus, one has

$$\sum_k \Omega_k^\pm \Omega_k^{\pm *} = P_{\mathrm{ac}}(H), \tag{44}$$

which implies that the full Møller operators

$$\Omega^\pm : \mathfrak{h} \ni u \mapsto \sum_k \Omega_k^\pm 1_k u,$$

is a partial isometry with initial space $\mathfrak{h}_{\mathrm{ac}}(H_{\mathscr{S}} \oplus H_{\mathscr{R}}) = \oplus_k \mathfrak{h}_{\mathrm{ac}}(H_k)$ and final space $\mathfrak{h}_{\mathrm{ac}}(H) = \mathfrak{h}$. The scattering operator $S = \Omega^{+*}\Omega^- : \oplus_k \mathfrak{h}_{\mathrm{ac}}(H_k) \to \oplus_k \mathfrak{h}_{\mathrm{ac}}(H_k)$ has a block matrix structure $S = [S_{jk}]$ where

$$S_{jk} = \Omega_j^{+*} \Omega_k^- : \mathfrak{h}_{\mathrm{ac}}(H_k) \to \mathfrak{h}_{\mathrm{ac}}(H_j).$$

It follows from Eq. (42) and (44) that

$$(S^* S)_{jk} = \sum_l (\Omega_l^{+*} \Omega_j^-)^* \Omega_l^{+*} \Omega_k^- = \Omega_j^{-*} \left(\sum_l \Omega_l^+ \Omega_l^{+*} \right) \Omega_k^- = \Omega_j^{-*} \Omega_k^- = \delta_{jk} P_{\mathrm{ac}}(H_k),$$

which shows that S is unitary.

3.4.4 The NESS

Fix $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_M) \in \mathbb{R}_+^M$, $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_M) \in \mathbb{R}^M$ and set $T_k = (I + \mathrm{e}^{\beta_k (H_k - \mu_k)})^{-1}$. Let $T_{\mathscr{S}} \in \mathscr{B}(\mathfrak{h}_{\mathscr{S}})$ be such that $0 < T_{\mathscr{S}} < 1$. Then

$$T = T_{\mathscr{S}} \oplus T_{\mathscr{R}} = T_{\mathscr{S}} \oplus \left(\bigoplus_{j=1}^M T_k \right), \tag{45}$$

generates a modular, gauge invariant quasi-free state on $\mathscr{O}$ such that $\omega_T(A) = \omega_{T_k}(A)$ for all $A \in \mathscr{O}_{\mathscr{R}_k}$. It follows from Theorem 3.2 that ω_T describes a physical state of the joint system

$\mathscr{S}+\mathscr{R}$ in which each reservoir $\mathscr{R}_k$ is in thermal equilibrium at inverse temperature β_k and chemical potential μ_k.

Since T_k commutes with $\mathrm{e}^{\mathrm{i}tH_k}$ we may write

$$\begin{aligned}T_t = \mathrm{e}^{-\mathrm{i}tH} T \mathrm{e}^{\mathrm{i}tH} &= \mathrm{e}^{-\mathrm{i}tH} T_{\mathscr{S}} \mathrm{e}^{\mathrm{i}tH} + \sum_k \mathrm{e}^{-\mathrm{i}tH} J_k T_k J_k^* \mathrm{e}^{\mathrm{i}tH} \\ &= \mathrm{e}^{-\mathrm{i}tH} T_{\mathscr{S}} \mathrm{e}^{\mathrm{i}tH} + \sum_k \mathrm{e}^{-\mathrm{i}tH} J_k \mathrm{e}^{\mathrm{i}tH_k} T_k \mathrm{e}^{-\mathrm{i}tH_k} J_k^* \mathrm{e}^{\mathrm{i}tH},\end{aligned}$$

Since $T_{\mathscr{S}}$ is compact, it follows from the Riemann-Lebesgue lemma, Eq. (41) and (43) (recall that we assumed $\mathfrak{h}_{\mathrm{ac}}(H)=\mathfrak{h}$) that

$$\operatorname*{s-lim}_{t\to+\infty} T_t = \sum_k \Omega_k^- T_k \Omega_k^{-*} = \Omega^- T_{\mathscr{R}} \Omega^{-*}. \tag{46}$$

so that Relation (40) holds with $T^+ = \Omega^- T_{\mathscr{R}} \Omega^{-*}$.

Let us now make connection with the C^*-scattering approach of Section 3.3.3. For $f \in \mathfrak{h}$, one has

$$\tau_0^{-t} \circ \tau^t (a^\#(f)) = a^\#(J_{\mathscr{S}} \mathrm{e}^{-\mathrm{i}tH_{\mathscr{S}}} J_{\mathscr{S}}^* \mathrm{e}^{\mathrm{i}tH} f) + \sum_k a^\#(J_k \mathrm{e}^{-\mathrm{i}tH_k} J_k^* \mathrm{e}^{\mathrm{i}tH} f),$$

where $J_{\mathscr{S}}$ denotes the canonical injection $\mathfrak{h}_{\mathscr{S}} \to \mathfrak{h}$. The same argument as before and the continuity of the map $f \mapsto a^\#(f)$ yield

$$\lim_{t\to\infty} \tau_0^{-t} \circ \tau^t (a^\#(f)) = \sum_k a^\#(J_k W_k^- f) = a^\#(\Omega^{-*} f) = \Gamma(\Omega^-)^* a^\#(f) \Gamma(\Omega^-).$$

The uniform continuity of the $*$-automorphisms $\tau_0^{-t} \circ \tau^t$ and the density of polynomials in $a^\#$ in $\mathrm{CAR}(\mathfrak{h})$ imply that

$$\lim_{t\to\infty} \tau_0^{-t} \circ \tau^t (A) = \Gamma(\Omega^-)^* A \Gamma(\Omega^-),$$

holds for any $A \in \mathrm{CAR}(\mathfrak{h})$. Thus, the Møller morphism γ^+ exists and is given by the Bogoliubov morphism

$$\gamma^+(A) = \Gamma(\Omega^-)^* A \Gamma(\Omega^-).$$

Its range is $\mathrm{CAR}(\operatorname{Ran}\Omega^{-*}) = \mathrm{CAR}(\mathfrak{h}_{\mathscr{R}}) = \mathscr{O}_{\mathscr{R}}$. The NESS can be written as

$$\omega_{T^+}(A) = \omega_{T_{\mathscr{R}}}(\gamma^+(A)),$$

and it follows from Propositions 3.4, 3.5 that

$$\lim_{t\to\infty} \nu(\tau^t(A)) = \omega_{T^+}(A),$$

holds for all $A \in \mathscr{O}$ and all $\nu \in \mathscr{N}_{\omega_T}$. Note in particular that the NESS is independent of the initial state $T_{\mathscr{S}}$ of the sample. Note also that the above arguments extend without modification to the more general class of initial states ω_T such that $0 < T < I$ and $J_k^* T J_k = T_k$.

3.4.5 Flux observables

In the framework of quasi-free fermionic systems, the total energy of reservoir $\mathscr{R}_k$ can be identified with the operator $\mathrm{d}\Gamma(H_k)$ (here and in the following, an operator A_k acting on $\mathfrak{h}_k$ is identified with the operator $J_k A_k J_k^*$ which acts on $\mathfrak{h}$). The energy flux leaving reservoir $\mathscr{R}_k$ is thus given by

$$\Phi_k^{\mathrm{e}} = -\left.\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(H)}\mathrm{d}\Gamma(H_k)\mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(H)}\right|_{t=0} = -\mathrm{d}\Gamma(\mathrm{i}[H,H_k]).$$

Besides energy fluxes, we can also introduce particle fluxes. The number of particles in reservoir $\mathscr{R}_k$ being given by $\mathrm{d}\Gamma(1_k)$, the particle flux leaving this reservoir is

$$\Phi_k^{\mathrm{p}} = -\left.\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(H)}\mathrm{d}\Gamma(1_k)\mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(H)}\right|_{t=0} = -\mathrm{d}\Gamma(\mathrm{i}[H,1_k]).$$

We note that all these flux observables have the same structure: each of them has the form

$$\Phi_k = \mathrm{d}\Gamma(\phi_k), \tag{47}$$

where $\phi_k = -\mathrm{i}[H,Q_k]$ for a self-adjoint operator Q_k commuting with $H_{\mathscr{R}}$ and $H_{\mathscr{S}}$. Even though the second quantized charge $\mathscr{Q}_k = \mathrm{d}\Gamma(Q_k)$ does not belong to the algebra $\mathscr{O}$, one has

$$\phi_k = -\mathrm{i}[H_{\mathscr{S}} + H_{\mathscr{R}} + V, Q_k] = -\mathrm{i}[V,Q_k] = \big((\chi_k,\cdot)\varphi_k + (\varphi_k,\cdot)\chi_k\big),$$

where $\varphi_k = \mathrm{i}Q_k\delta_{0_k}$. Thus

$$\Phi_k = a^*(\varphi_k)a(\chi_k) + a^*(\chi_k)a(\varphi_k),$$

is a self-adjoint element of $\mathscr{O}$.

Conservation of energy and particle number are expressed by the identities

$$\sum_k \Phi_k^{\mathrm{e}} = \mathrm{d}\Gamma(\mathrm{i}[H, H_{\mathscr{S}} + v]), \qquad \sum_k \Phi_k^{\mathrm{p}} = \mathrm{d}\Gamma(\mathrm{i}[H, 1_{\mathscr{S}}]).$$

Indeed, since $\mathrm{d}\Gamma(H_{\mathscr{S}} + V)$ and $\mathrm{d}\Gamma(1_{\mathscr{S}})$ belong to $\mathscr{O}$, one has

$$\sum_k \nu(\Phi_k^{\mathrm{e}}) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\nu(\tau^t(\mathrm{d}\Gamma(H_{\mathscr{S}}+V)))\right|_{t=0} = 0, \qquad \sum_k \nu(\Phi_k^{\mathrm{p}}) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\nu(\tau^t(\mathrm{d}\Gamma(1_{\mathscr{S}})))\right|_{t=0} = 0, \tag{48}$$

for any τ-invariant state ν.

3.4.6 Entropy production

Since the NESS ω_{T^+} is independent of the initial state of the sample $\mathscr{S}$, let us assume that

$$T_{\mathscr{S}} = (1 + \mathrm{e}^{-K_{\mathscr{S}}})^{-1},$$

for some self-adjoint operator $K_{\mathscr{S}}$ commuting with $H_{\mathscr{S}}$. Then we can write $T = (1+\mathrm{e}^{-K})^{-1}$ with $K = K_{\mathscr{S}} \oplus K_{\mathscr{R}}$ and

$$K_{\mathscr{R}} = -\bigoplus_j \beta_j(H_j - \mu_j 1_j).$$

It follows that ω_T is a KMS state at inverse temperature $\beta = -1$ for the group of Bogoliubov automorphisms $\sigma^t(A) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(K)} A \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(K)}$. By Theorem 3.6, we have

$$\mathrm{Ent}(\omega_{T_t}|\omega_T) = \int_0^t \omega_{T_s}(\mathrm{d}\Gamma(\mathrm{i}[K,V]))\,\mathrm{d}s.$$

In the limit $t \to +\infty$, we obtain

$$\begin{aligned}
0 \le -\lim_{t\to+\infty} \frac{1}{t}\mathrm{Ent}(\omega_{T_t}|\omega_T) &= -\omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[K,V])) \\
&= -\omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[K_{\mathcal{S}},V])) + \sum_{j=1}^M \omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[\beta_j(H_j+\mu_j 1_j),V])) \\
&= -\omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[K_{\mathcal{S}},V])) - \sum_{j=1}^M \omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[H,\beta_j(H_j+\mu_j 1_j)])) \\
&= -\omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[K_{\mathcal{S}},V])) - \sum_{j=1}^M \beta_j \omega_{T^+}(\Phi_j^{\mathrm{h}}),
\end{aligned}$$

where $\Phi_j^{\mathrm{h}} = \Phi_j^{\mathrm{e}} - \mu_j \Phi_j^{\mathrm{p}}$ denotes the heat flux leaving the j-th reservoir. Since the resulting inequality is valid for any $K_{\mathcal{S}}$, we can conclude that $\omega_{T^+}(\mathrm{d}\Gamma(\mathrm{i}[K_{\mathcal{S}},V]))$ vanishes for any choice of $K_{\mathcal{S}}$. Thus, the total entropy flux $\sum_j \beta_j \Phi_j^{\mathrm{h}}$ entering the sample satisfies

$$\sum_{j=1}^M \beta_j \omega_{T^+}(\Phi_j^{\mathrm{h}}) \le 0.$$

It follows that the entropy production in the steady state is also independent of the choice of the initial state of the sample and satisfies the entropy balance equation

$$\mathrm{Ep}(\omega_{T^+}) = -\sum_{j=1}^M \beta_j \omega_{T^+}(\Phi_j^{\mathrm{h}}).$$

3.4.7 The Landauer-Büttiker formula

Until the end of the next section T is given by Eq. (45), Q_k stands for either H_k or 1_k and $\phi_k = -\mathrm{i}[H, Q_k]$.

Formula (46) allows us to compute the expectation of the current observable (47), associated to the charge Q_k, in the NESS ω_{T^+},

$$\omega_{T^+}(\Phi_k) = \mathrm{tr}_{\mathfrak{h}}(T^+\phi_k) = \sum_{j=1}^M \mathrm{tr}_{\mathfrak{h}_j}(T_j \Omega_j^{-*} \phi_k \Omega_j^-). \tag{49}$$

The celebrated Landauer-Büttiker formula expresses the right hand side of this identity in terms of the scattering matrix $S = [S_{jk}]$. To write down this formula, we shall now describe the spectral representations of the reference Hamiltonians H_k.

Eq. (37) defines unitary operators

$$U_k : \mathfrak{h}_k \to L^2([-1,1], \mathrm{d}\varepsilon), \tag{50}$$

such that $(U_k H_k u)(\varepsilon) = \varepsilon(U_k u)(\varepsilon)$. It follows that $(U_k T_k u)(\varepsilon) = (1+\mathrm{e}^{\beta_k(\varepsilon-\mu_k)})^{-1}(U_k u)(\varepsilon)$. Since the scattering matrix $S = [S_{jk}]$ satisfies $H_j S_{jk} = S_{jk} H_k$, there exists measurable functions $s_{jk}(\varepsilon)$ such that $(U_j S_{jk} u)(\varepsilon) = s_{jk}(\varepsilon)(U_k u)(\varepsilon)$ for almost all $\varepsilon \in [-1,1]$. The matrix $S(\varepsilon) = [s_{jk}(\varepsilon)]$ is the so called *on-shell scattering matrix* at energy ε.

The Landauer-Büttiker formula for the energy currents reads

$$\omega_{T^+}(\Phi_k^{\mathrm{e}}) = \sum_{j=1}^{M} \int_{-1}^{1} \mathscr{T}_{kj}(\varepsilon)\varepsilon \left(\frac{1}{1+\mathrm{e}^{\beta_k(\varepsilon-\mu_k)}} - \frac{1}{1+\mathrm{e}^{\beta_j(\varepsilon-\mu_j)}} \right) \frac{\mathrm{d}\varepsilon}{2\pi}, \tag{51}$$

where $\mathscr{T}_{kj}(\varepsilon) = |\delta_{kj} - s_{kj}(\varepsilon)|^2$ is the so called *transmittance matrix*. A similar formula holds for the particle current

$$\omega_{T^+}(\Phi_k^{\mathrm{p}}) = \sum_{j=1}^{M} \int_{-1}^{1} \mathscr{T}_{kj}(\varepsilon) \left(\frac{1}{1+\mathrm{e}^{\beta_k(\varepsilon-\mu_k)}} - \frac{1}{1+\mathrm{e}^{\beta_j(\varepsilon-\mu_j)}} \right) \frac{\mathrm{d}\varepsilon}{2\pi}. \tag{52}$$

It is instructive to recover the energy conservation identity (48) from Eq. (51). To this end, we remark that the unitarity of the S-matrix, $\sum_m \overline{s}_{mj}(\varepsilon) s_{mk}(\varepsilon) = \delta_{jk}$, implies the sum rule

$$\sum_j \left(\mathscr{T}_{kj}(\varepsilon) - \mathscr{T}_{jk}(\varepsilon) \right) = 0,$$

for almost every $\varepsilon \in [0,1]$ and every $k \in \{1,\dots,M\}$. The Landauer-Büttiker formula (51) thus yields

$$\sum_k \omega_{T^+}(\Phi_k^{\mathrm{e}}) = \sum_{j,k=1}^{M} \int_{-1}^{1} \left(\mathscr{T}_{kj}(\varepsilon) - \mathscr{T}_{jk}(\varepsilon) \right) \varepsilon \frac{1}{1+\mathrm{e}^{\beta_k(\varepsilon-\mu_k)}} \frac{\mathrm{d}\varepsilon}{2\pi} = 0. \tag{53}$$

The particle number conservation identity

$$\sum_k \omega_{T^+}(\Phi_k^{\mathrm{p}}) = 0, \tag{54}$$

follows similarly from Eq. (52).

A formula expressing the electric current through a sample connected to two electronic reservoirs in terms of scattering data was first proposed by Landauer [L1, L2]. Similar formulas for more than two reservoirs were obtained later by Fischer and Lee [FL], Langreth and Abrahams [LA] and Büttiker and his coworkers [BILP, B1, B2]. Anderson and Engquist [AE] and Sivan and Imry [SI] have also considered the case of energy transport. We refer to [Da, I, IL] for more exhaustive references to the enormous physical literature on the subject.

We note however that physicists usually assume relaxation to a unique NESS and derive their formula from this assumption. Mathematical proofs of relaxation to a unique NESS and of the related Landauer-Büttiker formula first appeared in [AJPP1] for a simple special case and in [AJPP2, N] in more general settings.

The Landauer-Büttiker formula can be used to compute the conductance matrix, and more generally the Onsager matrix which expresses the steady state energy/particle currents in terms of temperature and chemical potential differentials to first order in these differentials (linear response theory). Let $\overline{\beta}$ and $\overline{\mu}$ denote equilibrium values of the inverse temperature and chemical potential and denote by

$$X_j^{\mathrm{e}} = \overline{\beta} - \beta_j, \qquad X_j^{\mathrm{p}} = \beta_j \mu_j - \overline{\beta}\overline{\mu}, \tag{55}$$

the thermodynamic forces which describe departures from the equilibrium situation. The Onsager matrix $L = [L_{kj}^{\mathrm{ab}}]_{\mathrm{a,b}\in\{\mathrm{e,p}\}; j,k\in\{1,\ldots,M\}}$ is defined by

$$L_{kj}^{\mathrm{ab}} = \partial_{X_j^{\mathrm{b}}} \omega_{T^+}(\Phi_k^{\mathrm{a}})\Big|_{X=0},$$

where we have set $X = (X_1^{\mathrm{e}}, \ldots, X_M^{\mathrm{e}}, X_1^{\mathrm{p}}, \ldots, X_M^{\mathrm{p}}) \in \mathbb{R}^{2M}$. Thus, linear response to the thermodynamic forces X is given by

$$\omega_{T^+}(\Phi_k^{\mathrm{a}}) = \sum_{\mathrm{b},j} L_{kj}^{\mathrm{ab}} X_j^{\mathrm{b}} + \mathscr{O}(|X|^2).$$

Since the energy/particle number conservation identities (53)/(54) imply $\sum_k L_{kj}^{\mathrm{ab}} = 0$, one has

$$L_{jj}^{\mathrm{ab}} = -\sum_{k\neq j} L_{kj}^{\mathrm{ab}},$$

and it is a simple exercise to differentiate Eq. (51), (52) to obtain, for $j \neq k$,

$$\begin{aligned} L_{kj}^{\mathrm{ee}} &= \int_{-1}^{1} \mathscr{T}_{kj}(\varepsilon)\varepsilon^2 f_{\mathrm{eq}}(1-f_{\mathrm{eq}})\frac{\mathrm{d}\varepsilon}{2\pi}, & L_{kj}^{\mathrm{ep}} &= \int_{-1}^{1} \mathscr{T}_{kj}(\varepsilon)\varepsilon f_{\mathrm{eq}}(1-f_{\mathrm{eq}})\frac{\mathrm{d}\varepsilon}{2\pi}, \\ L_{kj}^{\mathrm{pe}} &= \int_{-1}^{1} \mathscr{T}_{kj}(\varepsilon)\varepsilon f_{\mathrm{eq}}(1-f_{\mathrm{eq}})\frac{\mathrm{d}\varepsilon}{2\pi}, & L_{kj}^{\mathrm{pp}} &= \int_{-1}^{1} \mathscr{T}_{kj}(\varepsilon) f_{\mathrm{eq}}(1-f_{\mathrm{eq}})\frac{\mathrm{d}\varepsilon}{2\pi}, \end{aligned} \tag{56}$$

where

$$f_{\mathrm{eq}}(\varepsilon) = \frac{1}{1 + \mathrm{e}^{\overline{\beta}(\varepsilon - \overline{\mu})}},$$

is the equilibrium Fermi-Dirac distribution. A first rigorous proof of these linearized Landauer-Büttiker formulas was obtained in [CJM].

The open system $\mathscr{S} + \mathscr{R}$ is time reversal invariant (TRI) if there exists an anti-unitary involution $\theta_{\mathscr{S}}$ on $\mathfrak{h}_{\mathscr{S}}$ such that $\theta_{\mathscr{S}} H_{\mathscr{S}} \theta_{\mathscr{S}}^* = H_{\mathscr{S}}$ and $\theta_{\mathscr{S}} \chi_k = \chi_k$. Let $\theta_{\mathscr{R}} = \oplus_k \theta_k$ where θ_k is the complex conjugation on $\mathfrak{h}_k = \ell^2(\mathbb{N})$. Then $\theta_k H_k \theta_k^* = H_k$ and $\theta = \theta_{\mathscr{S}} \oplus \theta_{\mathscr{R}}$ satisfies $\theta H \theta^* = H$. Thus $\theta_k \mathrm{e}^{\mathrm{i}tH_k} \theta_k^* = \mathrm{e}^{-\mathrm{i}tH_k}$ and $\theta \mathrm{e}^{\mathrm{i}tH} \theta^* = \mathrm{e}^{-\mathrm{i}tH}$ from which we conclude that

$$\theta \Omega_k^{\pm} \theta_k^* = \mathrm{s}-\lim_{t\to\pm\infty} \theta \mathrm{e}^{\mathrm{i}tH} J_k \mathrm{e}^{-\mathrm{i}tH_k} \theta_k^* = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{-\mathrm{i}tH} J_k \mathrm{e}^{\mathrm{i}tH_k} = \Omega_k^{\mp},$$

and hence

$$\theta_j S_{jk}\theta_k^* = \theta_j \Omega_j^{+*}\theta^*\theta\Omega_k^-\theta_k^* = (\theta\Omega_j^+\theta_j^*)^*\theta\Omega_k^-\theta_k^* = \Omega_j^{-*}\Omega_k^+ = S_{jk}^*.$$

Since the unitary map U_k defined in Eq. (37), (50) satisfies $(U_k\theta_k u)(\varepsilon) = \overline{(U_k u)(\varepsilon)}$, we conclude that the on-shell S-matrix $s(\varepsilon) = [s_{jk}(\varepsilon)]$ is symmetric, i.e., $s^*(\varepsilon) = \overline{s(\varepsilon)}$ for almost every $\varepsilon \in [-1,1]$.

If the system $\mathscr{S} + \mathscr{R}$ is TRI, then the transmittance matrix $\mathscr{T}(\varepsilon) = [\mathscr{T}_{jk}(\varepsilon)]$ is also symmetric, and the linearized Landauer-Büttiker formulas (56) imply the Onsager reciprocity relations

$$L_{kj}^{\mathrm{ab}} = L_{jk}^{\mathrm{ba}}. \tag{57}$$

We shall give a proof of the Landauer-Büttiker formulas (51), (52) based on the Levitov formula in the next section. In Section 6 we shall prove a more general form of these formulas under appropriate but physically reasonable hypotheses. As opposed to the proofs in [AJPP2, N] which use the abstract stationary approach to scattering theory, we shall work within the framework of geometric, time-dependent scattering theory.

3.4.8 Full counting statistics

The total charge transferred from reservoir $\mathscr{R}_k$ to the sample $\mathscr{S}$ during the time interval $[0,t]$ can be expressed as an integral of the corresponding current

$$\delta\mathscr{Q}_k(t) = -\left(\tau^t(\mathscr{Q}_k) - \mathscr{Q}_k\right) = \int_0^t \tau^s(\Phi_k)\,\mathrm{d}s.$$

Note that even though the second quantized charge $\mathscr{Q}_k$ does not belong to the algebra $\mathscr{O}$ (and $\omega_T(\tau^t(\mathscr{Q}_k))$ is generally infinite for all t), the charge transfer $\delta\mathscr{Q}_k(t)$ is a self-adjoint element of $\mathscr{O}$ and

$$\omega_T(\delta\mathscr{Q}_k(t)) = \int_0^t \omega_T(\tau^s(\Phi_k))\,\mathrm{d}s, \tag{58}$$

is finite for all t and satisfies

$$\begin{aligned}\lim_{t\to\infty}\frac{1}{t}\omega_T(\delta\mathscr{Q}_k(t)) &= \lim_{t\to\infty}\frac{1}{t}\int_0^t \omega_T(\tau^s(\Phi_k))\,\mathrm{d}s = \lim_{t\to\infty}\omega_T(\tau^t(\Phi_k))\\ &= \omega_{T^+}(\Phi_k) = \lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\omega_T(\delta\mathscr{Q}_k(t)).\end{aligned}$$

We note however that since the observable $\tau^s(\Phi_k)$ and $\tau^{s'}(\Phi_k)$ do not commute for $s \neq s'$, there is no obvious measurement process for the observable $\delta\mathscr{Q}_k(t)$. Moreover, $\delta\mathscr{Q}_k(t)$ does not commute with $\delta\mathscr{Q}_j(t)$ for $k \neq j$, making an exact joint measurement of the components of $\delta\mathscr{Q}(t) = (\delta\mathscr{Q}_1(t),\ldots,\delta\mathscr{Q}_M(t))$ impossible.

In this section we discuss a more satisfactory approach to the charge transfer problem and derive the Levitov formula which provides a complete description of the transport statistics in the long time limit. The reader should consult [BN, EHM] for a pedagogical introduction and references to the physics literature. More mathematically oriented discussions and applications to other models can be found in [dR1, dR2, DdRM, JOPP, JPP2].

Finite size approximation. Let us assume for a while that the sets $\mathscr{R}_k$ are finite lattices $\{0,1,\dots,R\}$ so that the one-particle Hilbert spaces $\mathfrak{h}_k = \ell^2(\mathscr{R}_k)$ and hence $\mathfrak{h}$ are finite dimensional. We also replace the one-particle Hamiltonians H_k with the discrete Dirichlet Laplacians on $\ell^2(\mathscr{R}_k)$. In this setup the second quantized charges form a commuting family $\mathscr{Q} = (\mathscr{Q}_1,\dots,\mathscr{Q}_M)$ of self-adjoint elements of $\mathscr{O} = \mathrm{CAR}(\mathfrak{h}) = \mathscr{B}(\Gamma^-(\mathfrak{h}))$. Thus, one can analyze charge transport by measuring the vector observable $\mathscr{Q}$ at time 0 and at the later time t. The results of these two measurements are elements q and q' of the joint spectrum $\mathrm{Sp}(\mathscr{Q}) = \mathrm{Sp}(\mathscr{Q}_1)\times\cdots\times\mathrm{Sp}(\mathscr{Q}_M)\subset\mathbb{R}^M$. The probability distribution of the charge differences $\delta q = q - q'$ obtained with this protocol is called full counting statistics (FCS) of the charge transport. To compute this distribution, we note that since the components of $\mathscr{Q}$ commute, there exists a spectral family $\{P_q\}_{q\in\mathrm{Sp}(\mathscr{Q})}$ of orthogonal projections such that

$$f(\mathscr{Q}) = \sum_{q\in\mathrm{Sp}(\mathscr{Q})} f(q)P_q,$$

for all functions $f:\mathrm{Sp}(\mathscr{Q})\to\mathbb{C}$. The probability for the measurement of $\mathscr{Q}$ at time 0 to yield the result q is given by $\omega_T(P_q)$. After the measurement, the state of the system is given by

$$\omega(\cdot) = \frac{\omega_T(P_q\cdot P_q)}{\omega_T(P_q)},$$

so that the probability for a subsequent measurement of $\mathscr{Q}$ at the later time t to yield q' is

$$\omega(\tau^t(P_{q'})) = \frac{\omega_T(P_q\tau^t(P_{q'})P_q)}{\omega_T(P_q)}.$$

Hence, the joint probability distribution of the pair (q,q') is given by the Bayes formula

$$\mathbb{P}_t(q,q') = \omega_T(P_q)\frac{\omega_T(P_q\tau^t(P_{q'})P_q)}{\omega_T(P_q)} = \omega_T\left(P_q\tau^t(P_{q'})P_q\right).$$

Following the argument leading to Eq. (38), one shows that for any $\alpha\in\mathbb{R}^M$,

$$\omega_T(\mathrm{e}^{\mathrm{i}\alpha\cdot\mathscr{Q}}A\mathrm{e}^{-\mathrm{i}\alpha\cdot\mathscr{Q}}) = \omega_{T_\alpha}(A),$$

where $T_\alpha = \mathrm{e}^{-\mathrm{i}\alpha\cdot Q}T\mathrm{e}^{\mathrm{i}\alpha\cdot Q}$, $Q = (Q_1,\dots,Q_M)$, $\alpha\cdot Q = \alpha_1Q_1+\cdots+\alpha_MQ_M$, and $\alpha\cdot\mathscr{Q} = \mathrm{d}\Gamma(\alpha\cdot Q)$. Since Q_k commutes with T_k for all k one has $T_\alpha = T$ and it follows that $\omega_T(\mathrm{e}^{\mathrm{i}\alpha\cdot\mathscr{Q}}A\mathrm{e}^{-\mathrm{i}\alpha\cdot\mathscr{Q}}) = \omega_T(A)$. Thus,

$$\mathrm{e}^{\mathrm{i}\alpha\cdot(q-q')}\omega_T(P_qAP_{q'}) = \omega_T(\mathrm{e}^{\mathrm{i}\alpha\cdot\mathscr{Q}}P_qAP_{q'}\mathrm{e}^{-\mathrm{i}\alpha\cdot\mathscr{Q}}) = \omega_T(P_qAP_{q'}),$$

and hence $\omega_T(P_qAP_{q'}) = 0$ for $q\neq q'$. Since $\sum_q P_q = I$, we get

$$\omega_T(P_qAP_q) = \omega_T(P_qA) = \omega_T(AP_q), \tag{59}$$

which allows us to write

$$\mathbb{P}_t(q,q') = \omega_T\left(P_q\tau^t(P_{q'})\right).$$

If f is a polynomial in M variables, then

$$\mathbb{E}_t(f(\delta q)) = \sum_{q,q'\in \mathrm{Sp}(\mathcal{Q})} \mathbb{P}_t(q,q')f\left(q-q'\right) = \omega_T\left(\mathbf{T}f\left(\mathcal{Q}-\tau^t(\mathcal{Q})\right)\right),$$

where the time ordered observable $\mathbf{T}f\left(\mathcal{Q}-\tau^t(\mathcal{Q})\right)$ is obtained by substituting X_k by $\mathcal{Q}_k$ and Y_k by $\tau^t(\mathcal{Q}_k)$ in the expansion

$$f(X-Y) = \sum_{\alpha,\beta} f_{\alpha,\beta} X_1^{\alpha_1}\cdots X_M^{\alpha_M} Y_1^{\beta_1}\cdots Y_M^{\beta_M}.$$

It follows in particular that

$$\mathbb{E}_t(\delta q_k) = \omega_T\left(\delta\mathcal{Q}_k(t)\right) = \int_0^t \omega_T(\tau^s(\Phi_k))\,\mathrm{d}s, \tag{60}$$

and, taking Eq. (59) into account,

$$\mathbb{E}_t(\delta q_k \delta q_j) = \omega_T\left(\delta\mathcal{Q}_k(t)\delta\mathcal{Q}_j(t)\right). \tag{61}$$

Thus the moments of order one and two of the family of random variables δq_k coincide with the corresponding moments of the observables $\delta\mathcal{Q}_k(t)$ in the state ω_T. We stress however that this is no more the case for higher moments, as shown by a simple calculation.

The full counting statistics is the distribution of $\delta q = q - q'$, that is

$$\mathbb{P}_t(\delta q) = \sum_{\substack{q,q'\in \mathrm{Sp}(\mathcal{Q})\\ q-q'=\delta q}} \mathbb{P}_t(q,q').$$

Its Laplace transform is given by

$$\begin{aligned}\mathbb{R}^M \ni \alpha \mapsto \chi_t(\alpha) &= \sum_{\delta q\in \mathrm{Sp}(\mathcal{Q})-\mathrm{Sp}(\mathcal{Q})} \mathbb{P}_t(\delta q)\mathrm{e}^{\alpha\cdot\delta q}\\ &= \sum_{q,q'\in \mathrm{Sp}(\mathcal{Q})} \omega_T\left(P_q\tau^t(P_{q'})\right)\mathrm{e}^{-\alpha\cdot(q'-q)} = \omega_T(\mathrm{e}^{\alpha\cdot\mathcal{Q}}\tau^t(\mathrm{e}^{-\alpha\cdot\mathcal{Q}})).\end{aligned} \tag{62}$$

The function $\chi_t(\alpha)$ is the moment generating function of the random variable δq, i.e.,

$$\mathbb{E}_t(\delta q_k) = \left.\frac{\partial\chi_t}{\partial\alpha_k}\right|_{\alpha=0}, \qquad \mathbb{E}_t(\delta q_k\delta q_j) = \left.\frac{\partial^2\chi_t}{\partial\alpha_k\partial\alpha_j}\right|_{\alpha=0},$$

etc.

Writing $\mathrm{e}^{\alpha\cdot\mathcal{Q}}\tau^t(\mathrm{e}^{-\alpha\cdot\mathcal{Q}}) = \Gamma(\mathrm{e}^{\alpha\cdot Q}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\alpha\cdot Q}\mathrm{e}^{-\mathrm{i}tH})$, it follows from Eq. (28) that

$$\chi_t(\alpha) = \det(I + T(\mathrm{e}^{\alpha\cdot Q}\mathrm{e}^{-\alpha\cdot Q_t} - I)),$$

where we have set $Q_t = \mathrm{e}^{\mathrm{i}tH}Q\mathrm{e}^{-\mathrm{i}tH}$ (with an obvious abuse of notation). Using the fact that Q commutes with T, some elementary algebraic manipulations lead to $\chi_t(\alpha) = \det(I + X_t(\alpha))$ where

$$X_t(\alpha) = T^{1/2}\mathrm{e}^{\alpha\cdot Q/2}\left(\mathrm{e}^{-\alpha\cdot Q_t} - \mathrm{e}^{-\alpha\cdot Q}\right)\mathrm{e}^{\alpha\cdot Q/2}T^{1/2}.$$

Note that $X_t(\alpha)$ is self-adjoint. Moreover, integrating its derivative w.r.t. t yields the integral representation

$$X_t(\alpha) = \int_0^t T^{1/2} \mathrm{e}^{\alpha\cdot Q/2} \mathrm{e}^{\mathrm{i}sH} \mathrm{i}[V, \mathrm{e}^{-\alpha\cdot Q}] \mathrm{e}^{-\mathrm{i}sH} \mathrm{e}^{\alpha\cdot Q/2} T^{1/2}\, \mathrm{d}s. \tag{63}$$

Thermodynamic limit. At this point, we can investigate the thermodynamic limit $R \to \infty$ of our model. We use a superscript $^{(R)}$ to denote the objects pertaining to the system with finite reservoirs of size R, e.g., $\mathfrak{h}^{(R)}$ is the one-particle Hilbert space of the system with finite reservoirs. Let J_R be the canonical injection of $\mathfrak{h}^{(R)}$ into the one-particle Hilbert space $\mathfrak{h}$ of the system with infinite reservoirs. We first note that the coupling $V^{(R)}$ is such that $J_R V^{(R)} J_R^* = V$. We also observe that

$$\mathrm{s}-\lim_{R\to\infty} J_R Q_k^{(R)} J_R^* = Q_k, \qquad (Q_k = H_k \text{ or } Q_k = 1_k),$$

from which we easily conclude that

$$\mathrm{s}-\lim_{R\to\infty} J_R \mathrm{e}^{\alpha\cdot Q^{(R)}} J_R^* = \mathrm{e}^{\alpha\cdot Q}, \qquad \mathrm{s}-\lim_{R\to\infty} J_R \mathrm{e}^{\mathrm{i}tH^{(R)}} J_R^* = \mathrm{e}^{\mathrm{i}tH}, \qquad \mathrm{s}-\lim_{R\to\infty} J_R T^{(R)} J_R^* = T,$$

for any $\alpha \in \mathbb{C}^M$ and $t \in \mathbb{R}$. Rewriting Eq. (63) as

$$J_R X_t^{(R)}(\alpha) J_R^* = \int_0^t J_R T^{(R)1/2} \mathrm{e}^{\alpha\cdot Q^{(R)}/2} \mathrm{e}^{\mathrm{i}sH^{(R)}} \mathrm{i}[V, \mathrm{e}^{-\alpha\cdot Q^{(R)}}] \mathrm{e}^{-\mathrm{i}sH^{(R)}} \mathrm{e}^{\alpha\cdot Q^{(R)}/2} T^{(R)1/2} J_R^*\, \mathrm{d}s,$$

inserting the identity $I^{(R)} = J_R^* J_R$ between each factors of the right hand side of this formula and using the fact that V is finite rank we obtain that

$$\begin{aligned} \lim_{R\to\infty} J_R X_t^{(R)}(\alpha) J_R^* &= \int_0^t T^{1/2} \mathrm{e}^{\alpha\cdot Q/2} \mathrm{e}^{\mathrm{i}sH} \mathrm{i}[V, \mathrm{e}^{-\alpha\cdot Q}] \mathrm{e}^{-\mathrm{i}sH} \mathrm{e}^{\alpha\cdot Q/2} T^{1/2}\, \mathrm{d}s \\ &= T^{1/2} \mathrm{e}^{\alpha\cdot Q/2} \left(\mathrm{e}^{-\alpha\cdot Q_t} - \mathrm{e}^{-\alpha\cdot Q}\right) \mathrm{e}^{\alpha\cdot Q/2} T^{1/2} = X_t(\alpha), \end{aligned} \tag{64}$$

holds in trace norm. This implies in particular that the right hand side of this identity is trace class, and it follows from the continuity property of the determinant (see e.g., Theorem 3.4 in [S]) that

$$\chi_t(\alpha) = \lim_{R\to\infty} \chi_t^{(R)}(\alpha) = \det(I + X_t(\alpha)).$$

Since the function $\alpha \mapsto \chi_t(\alpha)$ is continuous, this pointwise convergence implies that the FCS $\mathbb{P}_t^{(R)}$ converges weakly to a probability measure $\mathbb{P}_t$ on $\mathbb{R}^M$ such that

$$\int \mathrm{e}^{\alpha\cdot\delta q} \mathrm{d}\mathbb{P}_t(\delta q) = \chi_t(\alpha), \tag{65}$$

for all $\alpha \in \mathbb{C}^M$ (see, e.g., Theorem 26.3 and its Corollary in [Bi]). We call $\mathbb{P}_t$ the FCS of the model with infinite reservoirs. Note that Eq. (60) and (61) also survive the thermodynamic limit, i.e.,

$$\int \delta q_k\, \mathrm{d}\mathbb{P}_t(\delta q) = \left.\frac{\partial \chi_t}{\partial \alpha_k}\right|_{\alpha=0} = \omega_T(\delta \mathcal{Q}_k(t)), \tag{66}$$

$$\int \delta q_k \delta q_j\, \mathrm{d}\mathbb{P}_t(\delta q) = \left.\frac{\partial^2 \chi_t}{\partial \alpha_k \partial \alpha_j}\right|_{\alpha=0} = \omega_T(\delta \mathcal{Q}_k(t) \delta \mathcal{Q}_j(t)). \tag{67}$$

Large time limit. We shall now consider the large time asymptotics of the FCS. For $\alpha \in \mathbb{R}^M$, $t \in \mathbb{R}$ and $u \in \mathfrak{h}$ one has

$$\begin{aligned}(u,(I+X_t(\alpha))u) &= (u,(I-T)u) + (u, T^{1/2}\mathrm{e}^{\alpha\cdot Q/2}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\alpha\cdot Q}\mathrm{e}^{-\mathrm{i}tH}\mathrm{e}^{\alpha\cdot Q/2}T^{1/2}u)\\ &\geq (u,(I-T)u) + \mathrm{e}^{-\sup \mathrm{Sp}(\alpha\cdot Q)}(u, T^{1/2}\mathrm{e}^{\alpha\cdot Q}T^{1/2}u)\\ &\geq (u,(I-T)u) + \mathrm{e}^{-\sup \mathrm{Sp}(\alpha\cdot Q)+\inf \mathrm{Sp}(\alpha\cdot Q)}(u,Tu)\\ &\geq (u,(I-(1-\kappa(\alpha))T)u)\\ &\geq \|u\|^2 - (1-\kappa(\alpha))(u,Tu) \geq \|u\|^2 - (1-\kappa(\alpha))\|u\|^2 = \kappa(\alpha)\|u\|^2,\end{aligned}$$

where $\kappa(\alpha) = \mathrm{e}^{\inf \mathrm{Sp}(\alpha\cdot Q)-\sup \mathrm{Sp}(\alpha\cdot Q)} \in]0,1]$. It follows that $I+\gamma X_t(\alpha) \geq \kappa(\alpha) > 0$ for $\gamma \in [0,1]$ and hence that

$$\frac{\mathrm{d}}{\mathrm{d}\gamma}\log\det(I+\gamma X_t(\alpha)) = \frac{\mathrm{d}}{\mathrm{d}\gamma}\mathrm{tr}\log(I+\gamma X_t(\alpha)) = \mathrm{tr}\left((I+\gamma X_t(\alpha))^{-1}X_t(\alpha)\right).$$

Using Eq. (64), the cyclicity of the trace and a change of integration variable allow us to write

$$\begin{aligned}\frac{1}{t}\log\chi_t(\alpha) &= \frac{1}{t}\int_0^1 \mathrm{d}\gamma \int_0^t \mathrm{d}s\,\mathrm{tr}\left((I+\gamma X_t(\alpha))^{-1}T^{1/2}\mathrm{e}^{\alpha\cdot Q/2}\mathrm{e}^{\mathrm{i}sH}\mathrm{i}[V,\mathrm{e}^{-\alpha\cdot Q}]\mathrm{e}^{-\mathrm{i}sH}\mathrm{e}^{\alpha\cdot Q/2}T^{1/2}\right)\\ &= \int_0^1 \mathrm{d}\gamma\int_0^1 \mathrm{d}s\,\mathrm{tr}\left(Y_t(s,\alpha,\gamma)\mathrm{i}[V,\mathrm{e}^{-\alpha\cdot Q}]\right),\end{aligned}$$

where $Y_t(s,\alpha,\gamma) = \mathrm{e}^{-\mathrm{i}tsH}\mathrm{e}^{\alpha\cdot Q/2}T^{1/2}(I+\gamma X_t(\alpha))^{-1}T^{1/2}\mathrm{e}^{\alpha\cdot Q/2}\mathrm{e}^{\mathrm{i}tsH}$ is easily seen to satisfy the estimate

$$\|Y_t(s,\alpha,\gamma)\| \leq \mathrm{e}^{2\sup \mathrm{Sp}(\alpha\cdot Q)-\inf \mathrm{Sp}(\alpha\cdot Q)}. \tag{68}$$

Elementary manipulations further yield

$$\begin{aligned}Y_t(s,\alpha,\gamma) &= \left(\mathrm{e}^{-\mathrm{i}tsH}\mathrm{e}^{-\alpha\cdot Q/2}T^{-1/2}(I+\gamma X_t(\alpha))T^{-1/2}\mathrm{e}^{-\alpha\cdot Q/2}\mathrm{e}^{\mathrm{i}tsH}\right)^{-1}\\ &= \left(\mathrm{e}^{-\mathrm{i}tsH}\mathrm{e}^{-\alpha\cdot Q}(T^{-1}-\gamma)\mathrm{e}^{\mathrm{i}tsH} + \gamma\mathrm{e}^{\mathrm{i}t(1-s)H}\mathrm{e}^{-\alpha\cdot Q}\mathrm{e}^{-\mathrm{i}t(1-s)H}\right)^{-1},\end{aligned}$$

and repeating the argument leading to Eq. (46), we can write

$$\begin{aligned}&\operatorname*{s-lim}_{t\to+\infty}\left(\mathrm{e}^{-\mathrm{i}tsH}\mathrm{e}^{-\alpha\cdot Q}(T^{-1}-\gamma)\mathrm{e}^{\mathrm{i}tsH} + \gamma\mathrm{e}^{\mathrm{i}t(1-s)H}\mathrm{e}^{-\alpha\cdot Q}\mathrm{e}^{-\mathrm{i}t(1-s)H}\right)\\ &\qquad= \Omega^-\mathrm{e}^{-\alpha\cdot Q}(T_{\mathscr{R}}^{-1}-\gamma)\Omega^{-*} + \gamma\Omega^+\mathrm{e}^{-\alpha\cdot Q}\Omega^{+*}\\ &\qquad= \Omega^-\left(\mathrm{e}^{-\alpha\cdot Q}(T_{\mathscr{R}}^{-1}-\gamma) + \gamma\Omega^{-*}\Omega^+\mathrm{e}^{-\alpha\cdot Q}\Omega^{+*}\Omega^-\right)\Omega^{-*}\\ &\qquad= \Omega^-\left(\mathrm{e}^{-\alpha\cdot Q}(T_{\mathscr{R}}^{-1}-\gamma) + \gamma S^*\mathrm{e}^{-\alpha\cdot Q}S\right)\Omega^{-*},\end{aligned}$$

for $s \in]0,1[$. The estimate (68) allows us to conclude that

$$\operatorname*{s-lim}_{t\to+\infty} Y_t(s,\alpha,\gamma) = \Omega^-\left(\mathrm{e}^{-\alpha\cdot Q}(T_{\mathscr{R}}^{-1}-\gamma)+\gamma S^*\mathrm{e}^{-\alpha\cdot Q}S\right)^{-1}\Omega^{-*} = \Omega^- Y(\alpha,\gamma)\Omega^{-*},$$

and an elementary calculation shows that

$$Y(\alpha,\gamma) = \left(\mathrm{e}^{-\alpha\cdot Q}(T_{\mathscr{R}}^{-1}-\gamma)+\gamma S^*\mathrm{e}^{-\alpha\cdot Q}S\right)^{-1} = \left(I+\gamma T_{\mathscr{R}}(\mathrm{e}^{\alpha\cdot Q}S^*\mathrm{e}^{-\alpha\cdot Q}S - I)\right)^{-1}T_{\mathscr{R}}\mathrm{e}^{\alpha\cdot Q}.$$

It follows that

$$\begin{aligned}\lim_{t\to+\infty}\frac{1}{t}\log\chi_t(\alpha) &= \int_0^1\int_0^1 \operatorname{tr}\left(\Omega^- Y(\alpha,\gamma)\Omega^{-*}\mathrm{i}[V,\mathrm{e}^{-\alpha\cdot Q}]\right)\mathrm{d}s\mathrm{d}\gamma\\ &= \int_0^1 \operatorname{tr}_{\mathfrak{h}_{\mathscr{R}}}\left(Y(\alpha,\gamma)\Omega^{-*}\mathrm{i}[V,\mathrm{e}^{-\alpha\cdot Q}]\Omega^-\right)\mathrm{d}\gamma.\end{aligned}$$

To evaluate the right hand side of this identity we need some technical results which we shall prove in Section 6.6. By Theorem 6.17, the finite rank operator C inside the trace has a integral representation

$$(U_jJ_j^*Cu)(\varepsilon)=\sum_k\int_{-1}^1 c_{jk}(\varepsilon,\varepsilon')(U_kJ_k^*u)(\varepsilon')\,d\varepsilon',$$

and its trace is given by

$$\operatorname{tr}_{\mathfrak{h}_{\mathscr{R}}}(C)=\sum_k\int_{-1}^1 c_{kk}(\varepsilon,\varepsilon)\,\mathrm{d}\varepsilon. \tag{69}$$

Moreover, by Lemma 6.19,

$$\sum_{jk}\int_{-1}^1 \overline{(U_jJ_j^*u)(\varepsilon)}c_{jk}(\varepsilon,\varepsilon)(U_kJ_k^*w)(\varepsilon)\,\mathrm{d}\varepsilon=\lim_{\eta\downarrow 0}\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u,\mathrm{e}^{-\mathrm{i}tH_{\mathscr{R}}}C\mathrm{e}^{\mathrm{i}tH_{\mathscr{R}}}w)\,\mathrm{d}t, \tag{70}$$

holds for u,w in a dense subspace of $\mathfrak{h}_{\mathscr{R}}$. The intertwining property of the Møller operator and the fact that Q commutes with $H_{\mathscr{S}}\oplus H_{\mathscr{R}}$ yield

$$\mathrm{e}^{-\mathrm{i}tH_{\mathscr{R}}}C\mathrm{e}^{\mathrm{i}tH_{\mathscr{R}}}=Y(\alpha,\gamma)\Omega^{-*}\mathrm{e}^{-\mathrm{i}tH}\mathrm{i}[V,\mathrm{e}^{-\alpha\cdot Q}]\mathrm{e}^{\mathrm{i}tH}\Omega^-=-\frac{\mathrm{d}}{\mathrm{d}t}Y(\alpha,\gamma)\Omega^{-*}\mathrm{e}^{-\mathrm{i}tH}\mathrm{e}^{-\alpha\cdot Q}\mathrm{e}^{\mathrm{i}tH}\Omega^-,$$

so that an integration by parts leads to the Abelian mean

$$\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u,\mathrm{e}^{-\mathrm{i}tH_{\mathscr{R}}}C\mathrm{e}^{\mathrm{i}tH_{\mathscr{R}}}w)\,\mathrm{d}t=\eta\int_0^{\infty}\mathrm{e}^{-\eta t}\left(u,Y(\alpha,\gamma)\Omega^{-*}(\mathrm{e}^{-\alpha\cdot Q_t}-\mathrm{e}^{-\alpha\cdot Q_{-t}})\Omega^-w\right)\mathrm{d}t.$$

Proceeding as above, we get

$$\mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{-\alpha\cdot Q_t}=\Omega^{\pm}\mathrm{e}^{-\alpha\cdot Q}\Omega^{\pm*},$$

and hence

$$\begin{aligned}\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u,\mathrm{e}^{-\mathrm{i}tH_{\mathscr{R}}}C\mathrm{e}^{\mathrm{i}tH_{\mathscr{R}}}w)\,\mathrm{d}t &= \left(u,Y(\alpha,\gamma)\Omega^{-*}(\Omega^+\mathrm{e}^{-\alpha\cdot Q}\Omega^{+*}-\Omega^-\mathrm{e}^{-\alpha\cdot Q}\Omega^{-*})\Omega^-w\right)\\ &= \left(u,Y(\alpha,\gamma)(S^*\mathrm{e}^{-\alpha\cdot Q}S-\mathrm{e}^{-\alpha\cdot Q})w\right)\\ &= \left(u,\left(I+\gamma T_{\mathscr{R}}(\mathrm{e}^{\alpha\cdot Q}S^*\mathrm{e}^{-\alpha\cdot Q}S-I)\right)^{-1}T_{\mathscr{R}}(\mathrm{e}^{\alpha\cdot Q}S^*\mathrm{e}^{-\alpha\cdot Q}S-I)w\right).\end{aligned}$$

Applying Lemma 6.18, Eq. (70) allows us to conclude that the $M\times M$ matrix $c(\varepsilon)=[c_{jk}(\varepsilon,\varepsilon)]$ is given by

$$c(\varepsilon)=\frac{1}{2\pi}\left(I+\gamma t(\varepsilon)(\mathrm{e}^{q(\alpha;\varepsilon)}s(\varepsilon)^*\mathrm{e}^{-q(\alpha;\varepsilon)}s(\varepsilon)-I)\right)^{-1}t(\varepsilon)(\mathrm{e}^{q(\alpha;\varepsilon)}s(\varepsilon)^*\mathrm{e}^{-q(\alpha;\varepsilon)}s(\varepsilon)-I),$$

where $t(\varepsilon)$ is the diagonal matrix with entries $t_{kk}(\varepsilon) = (1 + \mathrm{e}^{\beta_k(\varepsilon-\mu_k)})^{-1}$, $s(\varepsilon) = [s_{jk}(\varepsilon)]$ is the on-shell scattering matrix and $q(\alpha;\varepsilon) = \sum_k \alpha_k q_k(\varepsilon)$ is the diagonal matrix with entries

$$q_{kk}(\alpha;\varepsilon) = \begin{cases} \alpha_k & \text{for particle transport,} \\ \varepsilon\alpha_k & \text{for energy transport.} \end{cases}$$

Eq. (69) becomes

$$\mathrm{tr}_{\mathfrak{h}_{\mathscr{R}}}(C) = \int_{-1}^{1} \mathrm{tr}_{\mathbb{C}^M}(c(\varepsilon))\mathrm{d}\varepsilon = \int_{-1}^{1} \frac{\mathrm{d}}{\mathrm{d}\gamma}\mathrm{tr}_{\mathbb{C}^M}\log\left(I + \gamma t(\varepsilon)(\mathrm{e}^{q(\alpha;\varepsilon)}s(\varepsilon)^*\mathrm{e}^{-q(\alpha;\varepsilon)}s(\varepsilon) - I)\right)\frac{\mathrm{d}\varepsilon}{2\pi},$$

and integration over γ yields the Levitov formula [LL, LLL, Kl, ABGK, BN]

$$e_+(\alpha) = \lim_{t\to+\infty}\frac{1}{t}\log\chi_t(\alpha) = \int_{-1}^{1}\log\det{}_{\mathbb{C}^M}\left(I + t(\varepsilon)(\mathrm{e}^{q(\alpha;\varepsilon)}s(\varepsilon)^*\mathrm{e}^{-q(\alpha;\varepsilon)}s(\varepsilon) - I)\right)\frac{\mathrm{d}\varepsilon}{2\pi}. \tag{71}$$

Observing that $X_t(\alpha)$ is an entire analytic function of $\alpha \in \mathbb{C}^M$, it is not hard to show that the above limit holds for α in an open neighborhood of $\mathbb{R}^M$ in $\mathbb{C}^M$. Moreover, Eq. (65) and Hölder's inequality imply that the function $\mathbb{R}^M \ni \alpha \mapsto \log\chi_t(\alpha)$ is convex. Thus, the function $\mathbb{R}^M \ni \alpha \mapsto e_+(\alpha)$ is real analytic and convex. With $\mathbf{1} = (1,\dots,1) \in \mathbb{R}^M$ the matrix $q(\lambda\mathbf{1},\varepsilon)$ is a multiple of the identity for any $\lambda \in \mathbb{R}$ so that the function $e_+(\alpha)$ satisfies

$$e_+(\alpha + \lambda\mathbf{1}) = e_+(\alpha). \tag{72}$$

This property is clearly related to the conservation of energy/particle number and is an instance of the translation symmetry discussed in [AGMT] (see also [JPW, JPP2]).

Applications. 1. Our first application of Levitov formula is a derivation of the Landauer-Büttiker formulas. Eq. (66) and the convexity of the functions $t^{-1}\log\chi_t(\alpha)$ and $e_+(\alpha)$ imply that

$$\lim_{t\to+\infty}\mathbb{E}_t\left(\frac{\delta q_k}{t}\right) = \lim_{t\to+\infty}\frac{1}{t}\int\delta q_k\,\mathrm{d}\mathbb{P}_t(\delta q) = \lim_{t\to+\infty}\frac{\partial}{\partial\alpha_k}\frac{1}{t}\log\chi_t\bigg|_{\alpha=0} = \frac{\partial e_+}{\partial\alpha_k}\bigg|_{\alpha=0},$$

(see, e.g., Theorem 25.7 in [Ro]). Thus, it follows from Eq. (60) that

$$\omega_{T^+}(\Phi_k) = \lim_{t\to+\infty}\frac{1}{t}\int_0^t\omega_T(\tau^s(\Phi_k))\,\mathrm{d}s = \frac{\partial e_+}{\partial\alpha_k}\bigg|_{\alpha=0}.$$

It is a simple exercise to compute the derivative on the right hand side of this identity starting from the Levitov formula (71). The result of this calculation

$$\omega_{T^+}(\Phi_k) = \int_{-1}^{1}\mathrm{tr}_{\mathbb{C}^M}\left(t(\varepsilon)(s(\varepsilon)^*q_k(\varepsilon)s(\varepsilon) - q_k(\varepsilon))\right)\frac{\mathrm{d}\varepsilon}{2\pi},$$

is easily recognized to be the Landauer-Büttiker formulas (51), (52).

2. As a second application of Levitov formula, we show that it implies a large deviation principle which gives quantitative estimates for fluctuations of order 1 of the charge transfer rates

$\delta q_k/t$ around their mean values $\omega_{T^+}(\Phi_k)$ for large time. Applying the Gärtner-Ellis theorem (see, e.g., Theorem 2.3.6 in [DZ]), we conclude that the family of FCS $\{\mathbb{P}_t\}_{t\geq 0}$ satisfies a large deviation principle, i.e., for any Borel set $A\subset\mathbb{R}^M$, one has

$$-\inf_{q\in A^{\rm int}} I(q) \leq \liminf_{t\to+\infty}\frac{1}{t}\log\mathbb{P}_t\left(\frac{\delta q}{t}\in A\right) \leq \limsup_{t\to+\infty}\frac{1}{t}\log\mathbb{P}_t\left(\frac{\delta q}{t}\in A\right) \leq -\inf_{q\in A^{\rm cl}} I(q),$$

where $A^{\rm int}/A^{\rm cl}$ denotes the interior/closure of the set A and the rate function $I:\mathbb{R}^M\to[0,\infty[$ is the Legendre transform of e_+,

$$I(q) = \sup_{\alpha\in\mathbb{R}^M}\big(\alpha\cdot q - e_+(\alpha)\big).$$

It follows from Eq. (72) that $I(q)=+\infty$ unless $\mathbf{1}\cdot q = 0$, i.e., for any $a>0$ the probability $\mathbb{P}_t\left(\frac{\delta q}{t}\in A\right)$ decays more rapidly than e^{-at} as $t\to\infty$ unless the closure of A intersects the hyperplane $\mathscr{X}=\{q\in\mathbb{R}^M\,|\,\mathbf{1}\cdot q=0\}$ where the energy/particle number conservation is satisfied. It is therefore natural to decompose $\mathbb{R}^M=\mathscr{X}\oplus\mathbb{R}\mathbf{1}$ and rewrite the large deviation principle as

$$-\inf_{\hat q\in A^{\rm int}} I(\hat q) \leq \liminf_{t\to+\infty}\frac{1}{t}\log\mathbb{P}_t\left(\frac{\delta q}{t}\in A\oplus\mathbb{R}\mathbf{1}\right) \leq \limsup_{t\to+\infty}\frac{1}{t}\log\mathbb{P}_t\left(\frac{\delta q}{t}\in A\oplus\mathbb{R}\mathbf{1}\right) \leq -\inf_{\hat q\in A^{\rm cl}} I(\hat q),$$

for any Borel set $A\subset\mathscr{X}$. Roughly speaking, this means that

$$\mathbb{P}_t\left(\left\{\delta q\in\mathbb{R}^M\,\middle|\,\delta q - \left(\frac{1}{M}\sum_k\delta q_k\right)\mathbf{1}\simeq t\hat q\right\}\right)\simeq\mathrm{e}^{-tI(\hat q)},$$

for $\hat q\in\mathscr{X}$ and $t\to\infty$. One easily shows that $I(\hat q)\geq 0$ with equality if and and only if $\hat q = \omega_{T^+}(\Phi_k)$ (see, e.g. Lemma 2.3.9 in [DZ]).

3. Our third application of Levitov formula links FCS to linear response theory and more precisely to the Onsager matrix. We shall assume here that the system $\mathscr{S}+\mathscr{R}$ is TRI.

Applying the Levitov formula to the joint FCS $\mathbb{P}_t(q^{\rm e},q^{\rm p})$ of energy and particle transport which corresponds to the choice of commuting family $\mathscr{Q}=(\mathrm{d}\Gamma(h_1),\dots,\mathrm{d}\Gamma(h_M),\mathrm{d}\Gamma(1_1),\dots,\mathrm{d}\Gamma(1_M))$, we obtain a generating function

$$e_+(\alpha,\nu)=\lim_{t\to\infty}\frac{1}{t}\log\int\mathrm{e}^{\alpha\cdot\delta q^{\rm e}+\nu\cdot\delta q^{\rm p}}\,\mathrm{d}\mathbb{P}_t(\delta q^{\rm e},\delta q^{\rm p}),$$

given by

$$e_+(\alpha,\nu)=\int_{-1}^{1}\log\det\big(I+t(\varepsilon)(\mathrm{e}^{q(\alpha,\nu;\varepsilon)}s(\varepsilon)^*\mathrm{e}^{-q(\alpha,\nu\varepsilon)}s(\varepsilon)-I)\big)\frac{\mathrm{d}\varepsilon}{2\pi},$$

where $q(\alpha,\nu;\varepsilon)$ is the diagonal $M\times M$-matrix with entries $q_{kk}(\alpha,\nu;\varepsilon)=\alpha_k\varepsilon+\nu_k$. It follows that the translation symmetry

$$e_+(\alpha+\lambda\mathbf{1},\nu+\kappa\mathbf{1})=e_+(\alpha,\nu),$$

holds for all $\alpha,\nu\in\mathbb{R}^M$ and $\lambda,\kappa\in\mathbb{R}$.

We note that

$$t(\varepsilon)(I-t(\varepsilon))^{-1}=\mathrm{e}^{-\overline{\beta}(\varepsilon-\overline{\mu})}\mathrm{e}^{-q(X^{\mathrm{e}},X^{\mathrm{p}};\varepsilon)},$$

where X^{e} and X^{p} are the thermodynamic forces defined in Eq. (55). Writing the Levitov formula as

$$e_{+}(\alpha,\nu)=\int_{-1}^{1}\left[\log\det(I-t(\varepsilon))+\log\det\left(I+t(\varepsilon)(I-t(\varepsilon))^{-1}\mathrm{e}^{q(\alpha,\nu;\varepsilon)}s(\varepsilon)^{*}\mathrm{e}^{-q(\alpha,\nu;\varepsilon)}s(\varepsilon)\right)\right]\frac{\mathrm{d}\varepsilon}{2\pi},$$

and using the fact that TRI implies the symmetry of the scattering matrix, we observe that the second determinant on the right hand side is

$$\begin{aligned}
&\det\left(I+\mathrm{e}^{-\overline{\beta}(\varepsilon-\overline{\mu})}\ \mathrm{e}^{-q(X^{\mathrm{e}}-\alpha,X^{\mathrm{p}}-\nu;\varepsilon)}s^{*}(\varepsilon)\mathrm{e}^{-q(\alpha,\nu;\varepsilon)}s(\varepsilon)\right)\\
&\qquad=\det\left(I+\mathrm{e}^{-\overline{\beta}(\varepsilon-\overline{\mu})}\mathrm{e}^{-q(\alpha,\nu;\varepsilon)}s(\varepsilon)\mathrm{e}^{-q(X^{\mathrm{e}}-\alpha,X^{\mathrm{p}}-\nu;\varepsilon)}s(\varepsilon)^{*}\right)\\
&\qquad=\det\left(I+\mathrm{e}^{-\overline{\beta}(\varepsilon-\overline{\mu})}\mathrm{e}^{-q(\alpha,\nu;\varepsilon)}s^{*}(\varepsilon)\mathrm{e}^{-q(X^{\mathrm{e}}-\alpha,X^{\mathrm{p}}-\nu;\varepsilon)}s(\varepsilon)\right)\\
&\qquad=\det\left(I+\mathrm{e}^{-\overline{\beta}(\varepsilon-\overline{\mu})}\mathrm{e}^{-q(X^{\mathrm{e}},X^{\mathrm{p}};\varepsilon)}\mathrm{e}^{q(X^{\mathrm{e}}-\alpha,X^{\mathrm{p}}-\nu;\varepsilon)}s^{*}(\varepsilon)\mathrm{e}^{-q(X^{\mathrm{e}}-\alpha,X^{\mathrm{p}}-\nu;\varepsilon)}s(\varepsilon)\right),
\end{aligned}$$

which yields a quantum version of the generalized Evans-Searles symmetry

$$e_{+}(\alpha,\nu)=e_{+}(X^{\mathrm{e}}-\alpha,X^{\mathrm{p}}-\nu).$$

These symmetries play a central role in nonequilibrium statistical mechanics. The interested reader should consult [MR, JPR] for reviews of the classical theory and [K, dR1, DdRM, AGMT, JPW, JOPP, JPP2] for its adaptation to the quantum world. We also refer to [JOPS] for the link between the FCS of entropy production and the hypothesis testing of the arrow of time.

Since

$$\omega_{T^{+}}(\Phi_{k}^{\mathrm{e}})=\left.\frac{\partial e_{+}}{\partial\alpha_{k}}\right|_{\alpha=\nu=0},\qquad\omega_{T^{+}}(\Phi_{k}^{\mathrm{p}})=\left.\frac{\partial e_{+}}{\partial\nu_{k}}\right|_{\alpha=\nu=0},$$

one can write the Onsager matrix as

$$\begin{aligned}
L_{kj}^{\mathrm{ee}}&=\left.\frac{\partial^{2}e_{+}}{\partial X_{j}^{\mathrm{e}}\partial\alpha_{k}}\right|_{\alpha=\nu=0,X=0}, & L_{kj}^{\mathrm{ep}}&=\left.\frac{\partial^{2}e_{+}}{\partial X_{j}^{\mathrm{p}}\partial\alpha_{k}}\right|_{\alpha=\nu=0,X=0},\\
L_{kj}^{\mathrm{pe}}&=\left.\frac{\partial^{2}e_{+}}{\partial X_{j}^{\mathrm{e}}\partial\nu_{k}}\right|_{\alpha=\nu=0,X=0}, & L_{kj}^{\mathrm{pp}}&=\left.\frac{\partial^{2}e_{+}}{\partial X_{j}^{\mathrm{p}}\partial\nu_{k}}\right|_{\alpha=\nu=0,X=0}.
\end{aligned}\tag{73}$$

If a function $f(x,y)$ is C^{2} near $(x,y)=(0,0)\in\mathbb{R}^{M}\times\mathbb{R}^{M}$ and satisfies the symmetry $f(x,y)=f(x,x-y)$, then $(\partial_{y_k}f)(x,y)=-(\partial_{y_k}f)(x,x-y)$ and $(\partial_{x_j}\partial_{y_k}f)(x,y)=-(\partial_{x_j}\partial_{y_k}f)(x,x-y)-(\partial_{y_j}\partial_{y_k}f)(x,x-y)$ so that

$$(\partial_{x_j}\partial_{y_k}f)(0,0)=-\frac{1}{2}(\partial_{y_j}\partial_{y_k}f)(0,0).$$

Applying this result to the derivatives in Eq. (73), the translation symmetry and the generalized Evans-Searles symmetry yield the following linear response formulas

$$
\begin{aligned}
L_{kj}^{\mathrm{ee}} &= -\frac{1}{2}\frac{\partial^2 e_+}{\partial\alpha_j\partial\alpha_k}\bigg|_{\alpha=\nu=0,X=0}, &\qquad L_{kj}^{\mathrm{ep}} &= -\frac{1}{2}\frac{\partial^2 e_+}{\partial\nu_j\partial\alpha_k}\bigg|_{\alpha=\nu=0,X=0},\\
L_{kj}^{\mathrm{pe}} &= -\frac{1}{2}\frac{\partial^2 e_+}{\partial\alpha_j\partial\nu_k}\bigg|_{\alpha=\nu=0,X=0}, &\qquad L_{kj}^{\mathrm{pp}} &= -\frac{1}{2}\frac{\partial^2 e_+}{\partial\nu_j\partial\nu_k}\bigg|_{\alpha=\nu=0,X=0},
\end{aligned}
$$

where the right hand sides depend on the equilibrium FCS, i.e., on the function $e_+(\alpha,\nu)|_{X=0}$.

4. It is instructive to evaluate Levitov's formula for charge transport between 2 reservoirs $\mathscr{R}_L$, $\mathscr{R}_R$. In this situation the general form of the scattering matrix (i.e., of a unitary 2×2 matrix) is

$$
s(\varepsilon) = \begin{bmatrix} (1-\mathscr{T})^{1/2}\mathrm{e}^{\mathrm{i}\theta} & \mathscr{T}^{1/2}\mathrm{e}^{\mathrm{i}(\kappa-\eta)} \\ \mathscr{T}^{1/2}\mathrm{e}^{\mathrm{i}(\theta+\eta)} & -(1-\mathscr{T})^{1/2}\mathrm{e}^{\mathrm{i}\kappa} \end{bmatrix}
$$

where $\mathscr{T}\in[0,1]$ is the transmittance from one reservoir to the other and θ,κ,η are real phases, all depending on the energy ε. An elementary calculation leads to the following expression of Levitov's formula

$$
\begin{aligned}
e_+(\nu_L,\nu_R) &= \lim_{t\to\infty}\frac{1}{t}\log\int \mathrm{e}^{\nu_L\delta q_L^{\mathrm{p}}+\nu_R\delta q_R^{\mathrm{p}}}\,\mathrm{d}\mathbb{P}_t(\delta q_L^{\mathrm{p}},\delta q_R^{\mathrm{p}})\\
&= \int \log\left(p_0 + p_+\mathrm{e}^{(\nu_L-\nu_R)} + p_-\mathrm{e}^{-(\nu_L-\nu_R)}\right)\frac{\mathrm{d}\varepsilon}{2\pi},
\end{aligned}
$$

where

$$
p_+ = t_L(1-t_R)\mathscr{T},\qquad p_- = t_R(1-t_L)\mathscr{T},\qquad p_0 = 1-p_- - p_+.
$$

We note that, as a consequence of the translation symmetry (i.e., charge conservation), one has $e_+(\nu_L,\nu_R) = \hat{e}_+(\nu_L-\nu_R)$ where

$$
\hat{e}_+(\nu) = e_+(\nu,0) = \lim_{t\to\infty}\frac{1}{t}\log\int \mathrm{e}^{\nu\delta q_L^{\mathrm{p}}}\,\mathrm{d}\mathbb{P}_t(\delta q_L^{\mathrm{p}},\delta q_R^{\mathrm{p}}).
$$

If we further specialize to the zero temperature case ($\beta_L=\beta_R=+\infty$) then $t_L = 1_{]-\infty,\mu_L]}$, $t_R = 1_{]-\infty,\mu_R]}$ and assuming $\mu_R<\mu_L$, we get $p_-=0$ and $p_+ = 1_{]\mu_R,\mu_L]}\mathscr{T}$. It follows that

$$
\hat{e}_+(\nu) = \int_{\mu_R}^{\mu_L}\log\left(1-\mathscr{T}+\mathscr{T}\mathrm{e}^{\nu}\right)\frac{\mathrm{d}\varepsilon}{2\pi}.
$$

Neglecting the variation of the transmittance over the energy interval $[\mu_R,\mu_L]$ we finally obtain

$$
\hat{e}_+(\nu) = \frac{\Delta\mu}{2\pi}\log\left(1-\mathscr{T}+\mathscr{T}\mathrm{e}^{\nu}\right),
$$

with $\Delta\mu = \mu_L-\mu_R$. This can be interpreted in the following way. Let $(\xi_j)_{j\in\mathbb{N}^*}$ be a sequence of independent identically distributed random variables with values in $\{0,1\}$ and the law $\mathbb{P}(\xi_j = 1) = \mathscr{T}$. Set

$$
\Xi_t = \sum_{j=1}^{[t/\tau]}\xi_j,
$$

with $\tau = 2\pi/\Delta\mu$ (here $[\cdot]$ denotes the integer part). One easily computes

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\left(\mathrm{e}^{\nu\Xi_t}\right) = \hat{e}_+(\nu).$$

Thus, the Bernoulli process Ξ_t and the FCS of the charge transfer δq_L^{p} shares the same large deviations. Loosely speaking, ξ_j is the total charge transferred from the left reservoir to the right one in the time interval $[(j-1)\tau, j\tau]$ and the binomial law

$$\mathbb{P}_t(\delta q_L^{\mathrm{p}} = q) = \binom{t/\tau}{q} \mathcal{T}^q (1-\mathcal{T})^{t/\tau - q},$$

holds for large t (see, e.g., [BN]).

4 Commutators and Mourre Estimates

The commutator $[A,B] = AB - BA$ of two operators appears naturally in many problems of spectral theory and the use of commutators has a long history. Putnam's monograph [Pu] is a good introduction to the first results in this domain. The works of Mourre [M1, M2, M3] had a profound influence on the development of spectral analysis and scattering theory. They brought technical tools allowing for the proof of asymptotic completeness of the N-body problem which had been a struggle for decades [SS1, Gr, De1, SS2]. This section is a brief introduction to the elements of Mourre theory that we shall need in these notes. The monograph [ABG] provides a more detailed exposition (see also [DG] and [CFKS]).

4.1 Commutators

4.1.1 The commutator $[\cdot,\cdot]$ on $\mathcal{B}(\mathcal{H}) \times \mathcal{B}(\mathcal{H})$

If A and B are bounded operators on the Hilbert space $\mathcal{H}$ then their commutator $[A,B] = AB - BA$ is also a bounded operator. We may thus define the operator

$$\mathrm{ad}_A : B \mapsto \mathrm{i}[A,B],$$

on $\mathcal{B}(\mathcal{H})$. We note that ad_A is bounded with $\|\mathrm{ad}_A\| \le 2\,\|A\|$ so that $\theta \mapsto \tau_A^\theta = \mathrm{e}^{\theta\,\mathrm{ad}_A}$ is an entire function and

$$\frac{\mathrm{d}^k}{\mathrm{d}\theta^k} \tau_A^\theta(B) = \tau_A^\theta(\mathrm{ad}_A^k(B)),$$

and

$$\tau_A^\theta(B) = \sum_{k=0}^{\infty} \frac{\theta^k}{k!} \mathrm{ad}_A^k(B).$$

Note that $\tau_A^\theta(B) = \mathrm{e}^{\mathrm{i}\theta A} B \mathrm{e}^{-\mathrm{i}\theta A}$. If $A \in \mathcal{B}(\mathcal{H})$ is self-adjoint then ad_A is a $*$-derivation of the C^*-algebra $\mathcal{B}(\mathcal{H})$. In this case $\mathbb{R} \ni \theta \mapsto \mathrm{e}^{\mathrm{i}\theta\,\mathrm{ad}_A}$ is a real analytic (and thus strongly continuous) group of $*$-automorphisms of $\mathcal{B}(\mathcal{H})$.

4.1.2 The commutator $[A,\cdot]$ on $\mathscr{B}(\mathscr{H})$

Domain related problems make the definition of the commutator of two unbounded operators more delicate. However, Mourre theory which we shall need to develop the geometric scattering theory of quasi-free fermionic systems, is based on such commutators. In this section we discuss the definition of the commutator $[A,\cdot]$ with a self-adjoint operator A and its relation to the regularity of the group of $*$-automorphisms of $\mathscr{B}(\mathscr{H})$ generated by A.

Let A be a self-adjoint operator on the Hilbert space $\mathscr{H}$ with domain $\mathrm{Dom}(A)$. If $B \in \mathscr{B}(\mathscr{H})$ and if there exists a constant c such that

$$|(Au, Bu) - (u, BAu)| \le c\,\|u\|^2,$$

for all $u \in \mathrm{Dom}(A)$ then the sesquilinear form

$$\mathrm{Dom}(A) \times \mathrm{Dom}(A) \ni \langle u, v\rangle \mapsto (Au, Bv) - (u, BAv),$$

is continuous on a dense subspace of $\mathscr{H} \times \mathscr{H}$. Thus, it has a continuous extension to $\mathscr{H} \times \mathscr{H}$ and there exists an operator $C \in \mathscr{B}(\mathscr{H})$ such that

$$(Au, Bv) - (u, BAv) = (u, Cv),$$

for all $u, v \in \mathrm{Dom}(A)$. In this case we say that the commutator of A and B is bounded and we denote the operator C by the symbol $[A,B]$. If it is possible to iterate this construction we write

$$\mathrm{ad}_A^0 B \equiv B, \qquad \mathrm{ad}_A^k B \equiv \mathrm{i}[A, \mathrm{ad}_A^{k-1} B], (k = 1, 2, \dots).$$

Definition 4.1 *Let A be a self-adjoint operator on the Hilbert space $\mathscr{H}$. For each integer $n \ge 0$ we define*

$$\mathscr{B}_A^n(\mathscr{H}) \equiv \{B \in \mathscr{B}(\mathscr{H}) \,|\, \mathrm{ad}_A^k(B) \in \mathscr{B}(\mathscr{H}), k = 0, 1, \dots, n\}.$$

We remark that $\mathscr{B}_A^0(\mathscr{H}) = \mathscr{B}(\mathscr{H})$. We also write $\mathscr{B}_A(\mathscr{H}) \equiv \mathscr{B}_A^1(\mathscr{H})$.

The following characterization of $\mathscr{B}_A(\mathscr{H})$ will play an essential role.

Lemma 4.2 *Let A be a self-adjoint operator on the Hilbert space $\mathscr{H}$. For all $B \in \mathscr{B}(\mathscr{H})$ the following conditions are equivalent.*

(i) $B \in \mathscr{B}_A(\mathscr{H})$.

(ii) $B\mathrm{Dom}(A) \subset \mathrm{Dom}(A)$ *and there exists a constant c such that*

$$\|ABv - BAv\| \le c\|v\|, \tag{74}$$

for all $v \in \mathrm{Dom}(A)$.

(iii) $B^* \mathrm{Dom}(A) \subset \mathrm{Dom}(A)$ *and there exists a constant* c *such that*

$$\|B^* Au - AB^* u\| \leq c\|u\|, \tag{75}$$

for all $u \in \mathrm{Dom}(A)$.

When one of these conditions is satisfied, we have

$$[A,B]u = ABu - BAu, \qquad [A,B]^* u = B^* Au - AB^* u,$$

for all $u \in \mathrm{Dom}(A)$.

Proof. $(i) \Rightarrow (ii)$. Suppose $B \in \mathscr{B}_A(\mathscr{H})$ and set $C = [A,B]$. We have that $(Au, Bv) = (u, (BA + C)v)$ for all $u, v \in \mathrm{Dom}(A)$. Since A is self-adjoint, we deduce that $Bv \in \mathrm{Dom}(A)$ and that $(u, ABv) = (u, (BA+C)v)$. We thus have $B\mathrm{Dom}(A) \subset \mathrm{Dom}(A)$ and since $\mathrm{Dom}(A)$ is dense $Cv = ABv - BAv$ for all $v \in \mathrm{Dom}(A)$ and we can choose $c = \|C\|$ in (74).

$(ii) \Rightarrow (iii)$. If $B\mathrm{Dom}(A) \subset \mathrm{Dom}(A)$ and if (74) holds, then for all $u, v \in \mathrm{Dom}(A)$ we have that

$$(B^* u, Av) = (u, BAv) = (u, ABv) - (u, ABv - BAv) = (B^* Au, v) - (u, ABv - BAv).$$

We deduce that $|(B^* u, Av)| \leq (\|B\|\,\|Au\| + c\|u\|)\,\|v\|$, which allows us to conclude that $B^* u \in \mathrm{Dom}(A)$ and that $(AB^* u, v) - (B^* Au, v) = (u, ABv - BAv)$. In particular

$$|(AB^* u - B^* Au, v)| \leq c\|u\|\,\|v\|,$$

shows that (75) holds.

$(iii) \Rightarrow (i)$. If $B^* \mathrm{Dom}(A) \subset \mathrm{Dom}(A)$ and if (75) holds, then for all $u, v \in \mathrm{Dom}(A)$ we have

$$|(Au, Bv) - (u, BAv)| = |(B^* Au - AB^* u, v)| \leq c\,\|u\|\,\|v\|,$$

and thus $B \in \mathscr{B}_A(\mathscr{H})$.

Furthermore, since $\mathrm{Dom}(A)$ is dense in $\mathscr{H}$ we deduce from the fact that

$$(u, Cv) = (u, ABv - BAv) = (B^* Au - AB^* u, v) = (C^* u, v),$$

for all $u, v \in \mathrm{Dom}(A)$, that $Cv = ABv - BAv$ for all $v \in \mathrm{Dom}(A)$, and that $C^* u = B^* Au - AB^* u$ for all $u \in \mathrm{Dom}(A)$. □

Lemma 4.3 *Let* A *be a self-adjoint operator on the Hilbert space* $\mathscr{H}$ *and let* $n \geq 1$.

(i) $\mathscr{B}_A^n(\mathscr{H})$ *is a* $*$*-subalgebra of* $\mathscr{B}(\mathscr{H})$.

(ii) $\mathrm{ad}_A \colon \mathscr{B}_A^n(\mathscr{H}) \to \mathscr{B}_A^{n-1}(\mathscr{H})$ *is a* $*$*-derivation.*

Proof. It is obvious that $\mathscr{B}^n_A(\mathscr{H})$ is a subspace of $\mathscr{B}(\mathscr{H})$ and that ad_A is linear. Let $\mathscr{C}$ be a $*$-subalgebra of $\mathscr{B}(\mathscr{H})$ and

$$\mathscr{C}_A \equiv \{B \in \mathscr{C} \,|\, \mathrm{ad}_A(B) \in \mathscr{B}(\mathscr{H})\}.$$

We show that $\mathscr{C}_A$ is a $*$-subalgebra of $\mathscr{B}(\mathscr{H})$ and that ad_A is a $*$-derivation on $\mathscr{C}_A$. The facts that $B \in \mathscr{C}_A$ implies $B^* \in \mathscr{C}_A$ and that

$$\mathrm{ad}_A(B^*) = (\mathrm{ad}_A(B))^*,$$

are immediate consequences of Lemma 4.2.

Let $B, C \in \mathscr{C}_A$. By Lemma 4.2, B and C preserve $\mathrm{Dom}(A)$. Thus so does BC. For all $u \in \mathrm{Dom}(A)$ we also have $ABu - BAu = [A,B]u$ and $ACu - CAu = [A,C]u$. Thus,

$$ABCu - BCAu = [A,B]Cu + A[B,C]u,$$

and therefore

$$\|ABCu - BCAu\| \le (\|[A,B]\|\,\|C\| + \|A\|\,\|[B,C]\|)\,\|u\|.$$

Lemma 4.2 allows us to conclude that $BC \in \mathscr{C}_A$ and that $\mathrm{ad}_A(BC) = \mathrm{ad}_A(B)C + B\,\mathrm{ad}_A(C)$.

The proof of the lemma now follows by induction on n, noting that

$$\mathscr{B}^n_A(\mathscr{H}) = \{B \in \mathscr{B}^{n-1}_A(\mathscr{H}) \,|\, \mathrm{ad}_A(B) \in \mathscr{B}(\mathscr{H})\}.$$

□

The following result relates the iterated commutators ad^k_A to the regularity of the group of $*$-automorphisms

$$\tau^\theta_A(B) \equiv \mathrm{e}^{\mathrm{i}\theta A} B \mathrm{e}^{-\mathrm{i}\theta A},$$

generated by A. To formulate it, we make the following definition.

Definition 4.4 *Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$. An operator $B \in \mathscr{B}(\mathscr{H})$ is of class $C^n(A)$ if, for all $u \in \mathscr{H}$, the function*

$$\begin{array}{ccc} \mathbb{R} & \to & \mathscr{H} \\ \theta & \mapsto & \tau^\theta_A(B)u, \end{array}$$

is of class $C^n(\mathbb{R})$ in the norm topology of $\mathscr{H}$.

Lemma 4.5 *Let A be a self-adjoint operator and B a bounded operator on the Hilbert space $\mathscr{H}$. The following conditions are equivalent.*

(i) $B \in \mathscr{B}^n_A(\mathscr{H})$.

(ii) B *and* B^* *are of class* $C^n(A)$.

If one of these conditions is satisfied, then

$$\frac{\mathrm{d}^k}{\mathrm{d}\theta^k}\tau_A^\theta(B)u=\tau_A^\theta(\mathrm{ad}_A^k(B))u,$$

for all $u\in\mathcal{H}$ *and* $k\in\{0,1,\dots,n\}$.

Proof. $(ii)\Rightarrow(i)$ If $\theta\mapsto\tau_A^\theta(B)u$ and $\theta\mapsto\tau_A^\theta(B^*)u$ are of class C^n for all $u\in\mathcal{H}$ then

$$\lim_{h\to 0}\frac{\tau_A^h(B)u-Bu}{h}=Du,\qquad \lim_{h\to 0}\frac{\tau_A^h(B^*)u-B^*u}{h}=\tilde{D}u,$$

define two linear operators $D,\tilde{D}:\mathcal{H}\to\mathcal{H}$. Furthermore, for all $u,v\in\mathcal{H}$, we have

$$(v,Du)=\lim_{h\to 0}\frac{(v,\tau_A^h(B)u-Bu)}{h}=\lim_{h\to 0}\frac{(\tau_A^h(B^*)v-B^*v,u)}{h}=(\tilde{D}v,u),$$

that is to say that $D^*=\tilde{D}$. The Hellinger-Toeplitz theorem allows us to conclude that D is bounded. For $u\in\mathrm{Dom}(A)$

$$Du=\lim_{h\to 0}\mathrm{e}^{\mathrm{i}hA}B\frac{\mathrm{e}^{-\mathrm{i}hA}u-u}{h}+\frac{\mathrm{e}^{\mathrm{i}hA}Bu-Bu}{h}=-\mathrm{i}BAu+\lim_{h\to 0}\frac{\mathrm{e}^{\mathrm{i}hA}Bu-Bu}{h},$$

shows that $Bu\in\mathrm{Dom}(A)$ and $Du=\mathrm{i}ABu-\mathrm{i}BAu$. Lemma 4.2 allows us to conclude that $B\in\mathscr{B}_A(\mathcal{H})$ and $D=\mathrm{ad}_AB$.

If $u\in\mathcal{H}$ and $v=\mathrm{e}^{-\mathrm{i}\theta A}u$ then

$$\lim_{h\to 0}\frac{\tau_A^{\theta+h}(B)u-\tau_A^\theta(B)u}{h}=\lim_{h\to 0}\mathrm{e}^{\mathrm{i}\theta A}\frac{\tau_A^h(B)v-Bv}{h}=\mathrm{e}^{\mathrm{i}\theta A}Dv=\tau_A^\theta(D)u,$$

and it follows from our hypothesis that $\theta\mapsto\tau_A^\theta(D)u$ is of class C^{n-1}. A similar argument shows that the same is true for $\theta\mapsto\tau_A^\theta(D^*)u$. By iteration it is thus easy to conclude that

$$\frac{\mathrm{d}^k}{\mathrm{d}\theta^k}\tau_A^\theta(B)u=\tau_A^\theta\left(\mathrm{ad}_A^kB\right)u,$$

and that $\mathrm{ad}_A^kB\in\mathscr{B}(\mathcal{H})$ for $k=0,\dots,n$ and in particular that $B\in\mathscr{B}_A^n(\mathcal{H})$.

$(i)\Rightarrow(ii)$ Let $B\in\mathscr{B}_A^n(\mathcal{H})$. By Lemma 4.2, we have $B\mathrm{Dom}(A)\subset\mathrm{Dom}(A)$ and thus for all $u\in\mathrm{Dom}(A)$ we have

$$\tau_A^{\theta+h}(B)u-\tau_A^\theta(B)u=\int_0^1\frac{\mathrm{d}}{\mathrm{d}s}\mathrm{e}^{\mathrm{i}(\theta+sh)A}B\mathrm{e}^{-\mathrm{i}(\theta+sh)A}u\,\mathrm{d}s=h\int_0^1\mathrm{e}^{\mathrm{i}(\theta+sh)A}\mathrm{ad}_A(B)\mathrm{e}^{-\mathrm{i}(\theta+sh)A}u\,\mathrm{d}s.$$

This relation extends by continuity to all $u\in\mathcal{H}$. Furthermore, the strong continuity of the unitary group generated by A gives

$$\begin{aligned}\mathrm{e}^{\mathrm{i}(\theta+t)A}\mathrm{ad}_A(B)\mathrm{e}^{-\mathrm{i}(\theta+t)A}u=\tau_A^\theta\left(\mathrm{ad}_A(B)\right)u&+(\mathrm{e}^{\mathrm{i}(\theta+t)A}-\mathrm{e}^{\mathrm{i}\theta A})\mathrm{ad}_A(B)\mathrm{e}^{-\mathrm{i}\theta A}u\\&+\mathrm{e}^{\mathrm{i}(\theta+t)A}\mathrm{ad}_A(B)(\mathrm{e}^{-\mathrm{i}(\theta+t)A}-\mathrm{e}^{-\mathrm{i}\theta A})u\\&=\tau_A^\theta\left(\mathrm{ad}_A(B)\right)u+\mathrm{o}(1),\end{aligned}$$

as $t \to 0$. This allows us to write, for all $u \in \mathcal{H}$,

$$\frac{\tau_A^{\theta+h}(B)u - \tau_A^{\theta}(B)u}{h} = \int_0^1 \tau_A^{\theta+sh}(\mathrm{ad}_A(B))\, u\, \mathrm{d}s = \tau_A^{\theta}(\mathrm{ad}_A(B))\, u + \mathrm{o}(1).$$

We conclude that $\tau_A^{\theta}(B)u$ is of class C^1 and that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\tau_A^{\theta}(B)u = \tau_A^{\theta}(\mathrm{ad}_A(B))\, u,$$

with $\mathrm{ad}_A(B) \in \mathscr{B}_A^{n-1}(\mathcal{H})$. By iterating this argument we conclude that $\tau_A^{\theta}(B)u$ is of class C^n. Lemma 4.3 implies that $B^* \in \mathscr{B}_A^n(\mathcal{H})$ and we conclude that $\tau_A^{\theta}(B^*)u$ is also of class C^n. □

The next lemma provides a strong approximation result for iterated commutators in $\mathscr{B}_A^n(\mathcal{H})$.

Lemma 4.6 *Let A be a self-adjoint operator on the Hilbert space $\mathcal{H}$. For $\varepsilon \in \mathbb{R}^*$, we set*

$$A_\varepsilon \equiv \frac{\mathrm{e}^{\mathrm{i}\varepsilon A} - I}{\mathrm{i}\varepsilon} \in \mathscr{B}(\mathcal{H}).$$

For all $B \in \mathscr{B}(\mathcal{H})$, the two following conditions are equivalent.

(i) $B \in \mathscr{B}_A^n(\mathcal{H})$.

(ii) $\sup_{\varepsilon\in\mathbb{R}^*} \|\mathrm{ad}_{A_\varepsilon}^n(B)\| < \infty$.

If one of these conditions is satisfied then

$$\mathrm{s}-\lim_{\varepsilon\to 0} \mathrm{ad}_{A_\varepsilon}^n(B) = \mathrm{ad}_A^n(B).$$

Proof. One easily shows that

$$\varepsilon^{-1}(\tau_A^{\varepsilon} - \mathrm{Id})(B) = \mathrm{ad}_{A_\varepsilon}(B)\mathrm{e}^{-\mathrm{i}\varepsilon A},$$

from which one deduces

$$\varepsilon^{-n}(\tau_A^{\varepsilon} - \mathrm{Id})^n(B) = \mathrm{ad}_{A_\varepsilon}^n(B)\mathrm{e}^{-\mathrm{i}n\varepsilon A}. \tag{76}$$

Newton's formula

$$(\tau_A^{\varepsilon} - \mathrm{Id})^n = \sum_{k=0}^{n} \binom{n}{k} (-1)^{n-k} \tau_A^{k\varepsilon},$$

thus allows us to write, for all $u, v \in \mathcal{H}$,

$$(u, \mathrm{ad}_{A_\varepsilon}^n(B)v) = \sum_{k=0}^{n} \binom{n}{k} (-1)^{n-k} \varepsilon^{-n} (u, \tau_A^{k\varepsilon}(B)\mathrm{e}^{\mathrm{i}n\varepsilon A} v). \tag{77}$$

For all $u, v \in \mathrm{Dom}(A^\infty) \equiv \cap_{k>0}\mathrm{Dom}(A^k)$ the function

$$\mathbb{R} \ni \theta \mapsto (u, \tau_A^\theta(B)v) = (\mathrm{e}^{-\mathrm{i}\theta A}u, B\mathrm{e}^{-\mathrm{i}\theta A}v),$$

is of class C^∞ and thus admits a Taylor expansion around $\theta = 0$

$$(u, \tau_A^\theta(B)v) = \sum_{j=1}^{n-1} \frac{\theta^j}{j!} a_j(u,v) + \frac{\theta^n}{(n-1)!}\int_0^1 (1-s)^{n-1} a_n(\mathrm{e}^{-\mathrm{i}s\theta A}u, \mathrm{e}^{-\mathrm{i}s\theta A}v)\,\mathrm{d}s, \tag{78}$$

where a_j denotes the quadratic form defined on $\mathrm{Dom}(A^\infty) \times \mathrm{Dom}(A^\infty)$ by

$$a_j(u,v) \equiv \frac{\mathrm{d}^j}{\mathrm{d}\theta^j}(u, \tau_A^\theta(B)v)\bigg|_{\theta=0} = \frac{\mathrm{d}^j}{\mathrm{d}\theta^j}(\mathrm{e}^{-\mathrm{i}\theta A}u, B\mathrm{e}^{-\mathrm{i}\theta A}v)\bigg|_{\theta=0} = \mathrm{i}^j \sum_{l=0}^{j} \binom{j}{l}(-1)^l (A^{j-l}u, BA^l v). \tag{79}$$

Taking into account the fact that, for $j = 0, 1, \ldots, n-1$, we have

$$\sum_{k=0}^{n} \binom{n}{k}(-1)^{n-k}k^j = (x\partial_x)^j (x-1)^n\Big|_{x=1} = 0,$$

we obtain, after inserting the series (78) into (77), the formula

$$(u, \mathrm{ad}_{A_\varepsilon}^n(B)v) = \sum_{k=1}^{n}\binom{n}{k}(-1)^{n-k}\frac{nk^n}{n!}\int_0^1 (1-s)^{n-1} a_n(\mathrm{e}^{-\mathrm{i}ks\varepsilon A}u, \mathrm{e}^{\mathrm{i}(n-ks)\varepsilon A}v)\,\mathrm{d}s. \tag{80}$$

$(i) \Rightarrow (ii)$ If $B \in \mathscr{B}_A^n(\mathscr{H})$ then $\mathrm{ad}_A^n(B) \in \mathscr{B}(\mathscr{H})$. Lemma 4.5 implies that $\theta \mapsto \tau_A^\theta(B)u$ is of class C^n and that

$$a_n(u,v) = (u, \mathrm{ad}_A^n(B)v).$$

Formula (80) implies the bound

$$|(u, \mathrm{ad}_{A_\varepsilon}^n(B)v)| \le c\,\|u\|\,\|v\|\,\|\mathrm{ad}_A^n(B)\|,$$

for all $u, v \in \mathrm{Dom}(A^\infty)$ and a constant c. We deduce that

$$\sup_{\varepsilon\in\mathbb{R}^*}\|\mathrm{ad}_{A_\varepsilon}^n(B)\| < \infty,$$

and that, for all $v \in \mathscr{H}$,

$$\mathrm{ad}_{A_\varepsilon}^n(B)v = \sum_{k=1}^{n}\binom{n}{k}(-1)^{n-k}\frac{nk^n}{n!}\int_0^1 (1-s)^{n-1}\mathrm{e}^{\mathrm{i}ks\varepsilon A}\mathrm{ad}_A^n(B)\mathrm{e}^{\mathrm{i}(n-ks)\varepsilon A}v\,\mathrm{d}s.$$

It is then easy to conclude that

$$\lim_{\varepsilon\to 0}\mathrm{ad}_{A_\varepsilon}^n(B)v = \sum_{k=1}^{n}\binom{n}{k}(-1)^{n-k}\frac{k^n}{n!}\mathrm{ad}_A^n(B)v = \mathrm{ad}_A^n(B)v.$$

$(ii) \Rightarrow (i)$ Suppose that $\sup_{\varepsilon\in\mathbb{R}^*} \|\mathrm{ad}^n_{A_\varepsilon}(B)\| = c < \infty$. For all $u, v \in \mathrm{Dom}(A^\infty)$ we have

$$a_n(\mathrm{e}^{-\mathrm{i}ks\varepsilon A}u, \mathrm{e}^{\mathrm{i}(n-ks)\varepsilon A}v) = \mathrm{i}^n \sum_{j=0}^{n} \binom{n}{j} (-1)^j (\mathrm{e}^{-\mathrm{i}ks\varepsilon A}A^{n-j}u, B\mathrm{e}^{\mathrm{i}(n-ks)\varepsilon A}A^j v),$$

from which we deduce

$$\lim_{\varepsilon\to 0} a_n(\mathrm{e}^{-\mathrm{i}ks\varepsilon A}u, \mathrm{e}^{\mathrm{i}(n-ks)\varepsilon A}v) = a_n(u, v).$$

Formula (80) thus implies

$$a_n(u, v) = \lim_{\varepsilon\to 0}(u, \mathrm{ad}^n_{A_\varepsilon}(B)v),$$

and therefore

$$|a_n(u, v)| \le c\|u\|\,\|v\|.$$

Also, by writing the Taylor expansion (78) as

$$\sum_{j=0}^{n-1} \frac{\theta^j}{j!} a_j(u, v) = (u, \tau_A^\theta(B)v) - \frac{\theta^n}{(n-1)!}\int_0^1 (s-1)^{n-1} a_n(\mathrm{e}^{-\mathrm{i}s\theta A}u, \mathrm{e}^{-\mathrm{i}s\theta A}v)\,\mathrm{d}s,$$

we deduce that there exists constants c_j such that

$$|a_j(u, v)| \le c_j\,\|u\|\,\|v\|.$$

In particular

$$|a_1(u, v)| = |(Au, Bv) - (u, BAv)| \le c_1\,\|u\|\,\|v\|,$$

implies $B \in \mathscr{B}_A(\mathscr{H})$ and $a_1(u, v) = (u, \mathrm{ad}_A(B)v)$ by Lemma 4.2. We can finish the proof by induction. If $B \in \mathscr{B}^j_A(\mathscr{H})$ for $1 \le j < n$ then

$$|a_{j+1}(u, v)| = |(Au, \mathrm{ad}^j_A(B)v) - (u, \mathrm{ad}^j_A(B)Av)| \le c_{j+1}\|u\|\,\|v\|,$$

shows that $B \in \mathscr{B}^{j+1}_A(\mathscr{H})$. □

We finish this subsection with two results concerning the expansion of commutators which will be very useful to us later on. The first is purely algebraic whereas the second, a simple consequence of the Helffer-Sjöstrand formula, is due to [SiSo] (see also [HS]).

Lemma 4.7 *Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and $B \in \mathscr{B}^n_A(\mathscr{H})$. For all $z \in \mathrm{Res}(A)$ we have*

$$[(A-z)^{-n}, B] = \sum_{j=1}^{n} \binom{n}{j} \mathrm{i}^j (A-z)^{-j}\mathrm{ad}^j_A(B)(A-z)^{-n}. \tag{81}$$

Furthermore, $B\mathrm{Dom}(A^n) \subset \mathrm{Dom}(A^n)$ and in particular, $A^nB(A-z)^{-n} \in \mathscr{B}(\mathscr{H})$ for all $z \in \mathrm{Res}(A)$.

Proof. We prove (81) by induction on n. For $n=1$ we have

$$[(A-z)^{-1},B] = -(A-z)^{-1}[A,B](A-z)^{-1} = \binom{1}{1}\mathrm{i}(A-z)^{-1}\mathrm{ad}_A(B)(A-z)^{-1}.$$

For $1 \le k \le n$ we set

$$C_k \equiv \sum_{j=1}^{k}\binom{k}{j}\mathrm{i}^j(A-z)^{-j}\mathrm{ad}_A^j(B),$$

and we assume that $[(A-z)^{-k},B] = C_k(A-z)^{-k}$ for all integers k such that $1 \le k < n$.
We may thus write

$$\begin{aligned}
[(A-z)^{-k-1},B] &= [(A-z)^{-1}(A-z)^{-k},B] \\
&= (A-z)^{-1}[(A-z)^{-k},B] + [(A-z)^{-1},B](A-z)^{-k} \\
&= (A-z)^{-1}C_k(A-z)^{-k} + [(A-z)^{-1},B](A-z)^{-k} \\
&= C_k(A-z)^{-k-1} + [(A-z)^{-1},B+C_k](A-z)^{-k} \\
&= C_k(A-z)^{-k-1} - (A-z)^{-1}[A,B+C_k](A-z)^{-k-1} \\
&= \left(C_k - (A-z)^{-1}[A,B+C_k]\right)(A-z)^{-k-1},
\end{aligned}$$

and we easily verify that

$$C_k - (A-z)^{-1}[A,B+C_k] = C_{k+1},$$

which finishes the induction step.
By taking the adjoint, the identity (81) becomes

$$[B,(A-z)^{-n}] = \sum_{j=1}^{n}\binom{n}{j}(-\mathrm{i})^j(A-z)^{-n}\mathrm{ad}_A^j(B)(A-z)^{-j},$$

from which we deduce

$$(A-z)^nB(A-z)^{-n} = \sum_{j=0}^{n}\binom{n}{j}(-\mathrm{i})^j\mathrm{ad}_A^j(B)(A-z)^{-j}.$$

□

Theorem 4.8 *Let A be a self-adjoint operator on the Hilbert space $\mathscr{H}$, $B \in \mathscr{B}_A^n(\mathscr{H})$ and $f \in C^\infty(\mathbb{R})$ such that*

$$\|\!|f|\!\|_{n,k} \equiv \sum_{j=0}^{n}\sup_{x\in\mathbb{R}}|f^{(j)}(x)| + \sum_{j=n}^{k+2}\int\langle x\rangle^{j-n-1}|f^{(j)}(x)|\,\mathrm{d}x < \infty, \tag{82}$$

for some $k \ge n$. Then

$$[f(A),B] = \sum_{j=1}^{n}\frac{\mathrm{i}^j}{j!}f^{(j)}(A)\mathrm{ad}_A^j(B) + \mathscr{R}_n(f,A,B), \tag{83}$$

where the remainder is given by

$$\mathscr{R}_n(f,A,B) = \frac{1}{2\pi \mathrm{i}^{n+1}} \int \overline{\partial} \tilde{f}(z)(A-z)^{-n}[\mathrm{ad}_A^n(B),(A-z)^{-1}]\,\mathrm{d}\overline{z}\wedge \mathrm{d}z, \tag{84}$$

where $\tilde{f}$ is the almost-analytic extension of f of order k defined by (4). Furthermore, if $B \in \mathscr{B}_A^{n+1}(\mathscr{H})$, the remainder can also be written as

$$\mathscr{R}_n(f,A,B) = \frac{1}{2\pi \mathrm{i}^{n+2}} \int \overline{\partial} \tilde{f}(z)(A-z)^{-n-1}\mathrm{ad}_A^{n+1}(B)(A-z)^{-1}\,\mathrm{d}\overline{z}\wedge \mathrm{d}z.$$

Remark. By taking the adjoint we obtain a similar formula

$$[f(A),B] = -\sum_{j=1}^{n} \frac{(-\mathrm{i})^j}{j!}\mathrm{ad}_A^j(B) f^{(j)}(A) - \mathscr{R}_n(\overline{f},A,B^*)^*.$$

Proof. We first consider $f \in C_0^\infty(\mathbb{R})$. Let $\tilde{f}$ be the almost-analytic extension of order n given by (4). The Helffer-Sjöstrand formula (6) allows us to write

$$[f(A),B] = \frac{1}{2\pi\mathrm{i}} \int \overline{\partial} \tilde{f}(z)[B,(A-z)^{-1}]\,\mathrm{d}\overline{z}\wedge \mathrm{d}z.$$

A repeated use of the identity

$$\begin{aligned}
[\mathrm{ad}_A^j(B),(A-z)^{-1}] &= (A-z)^{-1}[A,\mathrm{ad}_A^j(B)](A-z)^{-1} \\
&= -\mathrm{i}(A-z)^{-1}\mathrm{ad}_A^{j+1}(B)(A-z)^{-1} \\
&= -\mathrm{i}(A-z)^{-2}\mathrm{ad}_A^{j+1}(B) - \mathrm{i}(A-z)^{-1}[\mathrm{ad}_A^{j+1}(B),(A-z)^{-1}],
\end{aligned}$$

and Formula (6) lead to

$$\begin{aligned}
[f(A),B] &= \sum_{j=1}^{n}\left(\frac{1}{2\pi\mathrm{i}}\int \overline{\partial}\tilde{f}(z)(A-z)^{-1-j}\,\mathrm{d}\overline{z}\wedge\mathrm{d}z\right)(-\mathrm{i})^j\mathrm{ad}_A^j(B) \\
&\quad + \frac{1}{2\pi\mathrm{i}^{n+1}}\int \overline{\partial}\tilde{f}(z)(A-z)^{-n}[\mathrm{ad}_A^n(B),(A-z)^{-1}]\,\mathrm{d}\overline{z}\wedge\mathrm{d}z \\
&= \sum_{j=1}^{n}\frac{\mathrm{i}^j}{j!}f^{(j)}(A)\mathrm{ad}_A^j(B) + \mathscr{R}_n(f,A,B),
\end{aligned}$$

where $\mathscr{R}_n$ is given by (84).

We now consider $f \in C^\infty(\mathbb{R})$ satisfying (82). Let $\varphi_m(x) \equiv \varphi(x/m)$ with $\varphi \in C_0^\infty(]-1,1[)$ being such that $0 \le \varphi \le 1$ and $\varphi(x) = 1$ for all $x \in [-1/2,1/2]$. Then $f_m \equiv f\varphi_m \in C_0^\infty(\mathbb{R})$, $\lim_m f_m^{(j)}(x) = f^{(j)}(x)$ for all $x \in \mathbb{R}$ and (82) imply that $\sup_{m,x\in\mathbb{R}} |f_m^{(j)}(x)| < \infty$ for all $j \in \{0,\dots,n\}$. The functional calculus allows us to conclude that $\mathrm{s}-\lim_m f_m^{(j)}(A) = f^{(j)}(A)$ and in particular that

$$\mathrm{s}-\lim_m [f_m(A),B] = [f(A),B].$$

The estimate (5) allows us to obtain, starting from the representation of the remainder (84),

$$\begin{aligned}\|\mathscr{R}_n(f,A,B)\| &\le \frac{\|\mathrm{ad}_A^n(B)\|}{\pi}\int |\bar\partial\tilde f(x+\mathrm{i}y)|\,|y|^{-n-1}\mathrm{d}\bar z\wedge\mathrm{d}z\\ &\le C\sum_{j=0}^{k+2}\int \langle x\rangle^{j-n-1}|f^{(j)}(x)|\,\mathrm{d}x.\end{aligned}$$

We deduce that

$$\|\mathscr{R}_n(f,A,B)-\mathscr{R}_n(f_m,A,B)\|\le C\int g_m(x)\,\mathrm{d}x,$$

where we have set

$$g_m(x)=\sum_{j=0}^{k+2}\langle x\rangle^{j-n-1}|f^{(j)}(x)-f_m^{(j)}(x)|.$$

Starting from the expansion

$$f^{(j)}(x)-f_m^{(j)}(x)=\sum_{l=0}^{j}\binom{j}{l}f^{(l)}(x)(\delta_{jl}-m^{-(j-l)}\varphi^{(j-l)}(x/m)),$$

we obtain the estimate

$$\begin{aligned}g_m(x)&\le\sum_{j=0}^{k+2}\langle x\rangle^{j-n-1}\sum_{l=0}^{j}\binom{j}{l}|f^{(l)}(x)||\delta_{jl}-m^{-(j-l)}\varphi^{(j-l)}(x/m)|\\ &\le\sum_{l=0}^{k+2}\langle x\rangle^{l-n-1}|f^{(l)}(x)|\sum_{j=l}^{k+2}\binom{j}{l}\langle x\rangle^{j-l}|\delta_{jl}-m^{-(j-l)}\varphi^{(j-l)}(x/m)|\\ &\le\sum_{l=0}^{k+2}\langle x\rangle^{l-n-1}|f^{(l)}(x)|\sum_{j=l}^{k+2}\binom{j}{l}(\delta_{jl}+\langle m\rangle^{j-l}m^{-(j-l)}\varphi^{(j-l)}(x/m))\\ &\le C'\sum_{l=0}^{k+2}\langle x\rangle^{l-n-1}|f^{(l)}(x)|\equiv g(x),\end{aligned}$$

and as (82) implies that $g\in L^1(\mathbb{R})$ we can apply the dominated convergence theorem to conclude that

$$\lim_m\mathscr{R}_n(f_m,A,B)=\mathscr{R}_n(f,A,B).$$

The identity (83), with $f=f_m$ is thus preserved in the limit $m\to\infty$, which proves (83) in the general case.

Finally, we note that if $B\in\mathscr{B}_A^{n+1}(\mathscr{H})$ the remainder $\mathscr{R}_n$ can also be written as

$$\begin{aligned}\mathscr{R}_n(f,A,B)&=\frac{1}{2\pi\mathrm{i}^{n+1}}\int\bar\partial\tilde f(z)(A-z)^{-n}[\mathrm{ad}_A^n(B),(A-z)^{-1}]\,\mathrm{d}\bar z\wedge\mathrm{d}z\\ &=\frac{1}{2\pi\mathrm{i}^{n+2}}\int\bar\partial\tilde f(z)(A-z)^{-n-1}\mathrm{ad}_A^{n+1}(B)(A-z)^{-1}\,\mathrm{d}\bar z\wedge\mathrm{d}z.\end{aligned}$$

□

4.1.3 The commutator of two self-adjoint operators

In this subsection we shall extend the discussion to commutators of type $[A,H]$ where A and H are self-adjoint operators on $\mathscr{H}$. We shall start by studying commutators of the form $[A,(H-z)^{-1}]$.

Lemma 4.9 *Let A be a self-adjoint operator and B a closed operator on the Hilbert space $\mathscr{H}$. Let $\mathrm{Res}(B)$ be the resolvent set of B and $R(z) \equiv (B-z)^{-1}$ its resolvent.*

(i) If $R(z_0) \in \mathscr{B}_A^n(\mathscr{H})$ for some $z_0 \in \mathrm{Res}(H)$ then $R(z) \in \mathscr{B}_A^n(\mathscr{H})$ for all $z \in \mathrm{Res}(B)$.

(ii) For all $z, z_0 \in \mathrm{Res}(B)$ we have

$$\mathrm{ad}_A(R(z)) = (I+(z-z_0)R(z))\mathrm{ad}_A(R(z_0))(I+(z-z_0)R(z)).$$

This relation allows for the inductive calculation of $\mathrm{ad}_A^k(R(z))$ for $k=2,\ldots,n$.

Proof. We set $R \equiv R(z)$, $R_0 \equiv R(z_0)$, and $w \equiv z-z_0$. The first resolvent equation $R-R_0 = wRR_0$ gives $(I-wR_0)^{-1} = I+wR$. With the notation from the proof of Lemma 4.6 we have, for $u \in \mathrm{Dom}(A)$,

$$\begin{aligned}(I+wR)Au &= \lim_{\varepsilon\to 0}(I+wR)A_\varepsilon u = \lim_{\varepsilon\to 0}(I+wR)A_\varepsilon(I-wR_0)(I+wR)u \\ &= \lim_{\varepsilon\to 0}\left(A_\varepsilon(I+wR)u - w(I+wR)[A_\varepsilon,R_0](I+wR)u\right).\end{aligned}$$

By applying Lemma 4.6 we obtain

$$\lim_{\varepsilon\to 0} A_\varepsilon(I+wR)u = w(I+wR)[A,R_0](I+wR)u + (I+wR)Au,$$

which shows that $(I+wR)u \in \mathrm{Dom}(A)$ and allows us to write

$$A(I+wR)u = w(I+wR)[A,R_0](I+wR)u + (I+wR)Au,$$

or alternatively

$$ARu - RAu = (I+wR)[A,R_0](I+wR)u.$$

Using Lemma 4.2 gives

$$[A,R] = (I+wR)[A,R_0](I+wR),$$

which shows (i) in the particular case where $n=1$ as well as (ii). To show (i) in the general case we proceed by induction on n. Suppose assertion (i) holds for $n \le m$ and that $R_0 \in \mathscr{B}_A^{m+1}(\mathscr{H})$. We then have that $R_0 \in \mathscr{B}_A^m(\mathscr{H})$ and the induction hypothesis allows us to state that $R \in \mathscr{B}_A^m(\mathscr{H})$. ad_A, being a derivation, satisfies the Leibniz formula

$$\mathrm{ad}_A^m(BC) = \sum_{k=0}^m \binom{m}{k} \mathrm{ad}_A^k(B)\,\mathrm{ad}_A^{(m-k)}(C).$$

Since $R = (I + wR)R_0$ we have

$$\mathrm{ad}_A^m(R) = \sum_{k=0}^{m} \binom{m}{k} \mathrm{ad}_A^k(I + wR)\,\mathrm{ad}_A^{(m-k)}(R_0),$$

which can also be written as

$$\mathrm{ad}_A^m(R)(I - wR_0) = \sum_{k=0}^{m-1} \binom{m}{k} \mathrm{ad}_A^k(I + wR)\,\mathrm{ad}_A^{(m-k)}(R_0),$$

or as

$$\mathrm{ad}_A^m(R) = \sum_{k=0}^{m-1} \binom{m}{k} \mathrm{ad}_A^k(I + wR)\,\mathrm{ad}_A^{(m-k)}(R_0)(I + wR). \tag{85}$$

We deduce that

$$\begin{aligned}\mathrm{ad}_A^{m+1}(R) = \sum_{k=0}^{m-1} \binom{m}{k} \Big[& w\,\mathrm{ad}_A^{k+1}(R)\,\mathrm{ad}_A^{(m-k)}(R_0)(I + wR) \\ & + \mathrm{ad}_A^k(I + wR)\,\mathrm{ad}_A^{(m+1-k)}(R_0)(I + wR) \\ & + w\,\mathrm{ad}_A^k(I + wR)\,\mathrm{ad}_A^{(m-k)}(R_0)\mathrm{ad}_A(R)\Big],\end{aligned}$$

and thus $R \in \mathscr{B}_A^{m+1}(\mathscr{H})$, which validates the induction step. □

Lemma 4.10 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$. If there exists $z_0 \in \mathrm{Res}(H)$ such that $(H - z_0)^{-1} \in \mathscr{B}_A^n(\mathscr{H})$ then $f(H) \in \mathscr{B}_A^n(\mathscr{H})$ for all $f \in C_0^\infty(\mathbb{R})$.*

Proof. We set $R(z) \equiv (H - z)^{-1}$ and $|||B|||_{A,n} \equiv \max_{k \le n} \|\mathrm{ad}_A^k B\|$ for $B \in B_A^n(\mathscr{H})$. Using Formula (85) we easily show that for $n \ge 1$

$$\left\|\mathrm{ad}_A^n R(z)\right\| \le (1 + |z - z_0|)^{n-1} \left(1 + \frac{|z - z_0|}{|\mathrm{Im}\, z|}\right)^{n+1} \left(n - 1 + |||R(z_0)|||_{A,n}\right)^n.$$

We may thus use the Helffer-Sjöstrand formula to obtain

$$\mathrm{ad}_A^n(f(H)) = \int_{\mathbb{C}} \bar\partial \tilde f(z)\,\mathrm{ad}_A^n R(z) \frac{\mathrm{d}z \wedge \mathrm{d}\bar z}{\pi}.$$

□

Definition 4.11 *Let A be a self-adjoint operator on the Hilbert space $\mathscr{H}$. A self-adjoint operator H on $\mathscr{H}$ is locally of class $C^n(A)$ (or of class $C^n_{\mathrm{loc}}(A)$) if $f(H)$ is of class $C^n(A)$ for all $f \in C_0^\infty(\mathbb{R})$.*

A self-adjoint operator H is thus of class $C^n_{\mathrm{loc}}(A)$ if, for all $u \in \mathscr{H}$ and for all $f \in C_0^\infty(\mathbb{R})$ the function $\mathbb{R} \ni \theta \to \tau_A^\theta(f(H))u = f(\tau_A^\theta(H))u$ is of class C^n. The following lemma is an immediate corollary of Lemmas 4.5 and 4.10.

Lemma 4.12 *Let A and H be self-adjoint operators on the Hilbert space $\mathcal{H}$. The two following conditions are equivalent.*

(i) H *is of class* $C^n_{\mathrm{loc}}(A)$.

(ii) *There exists* $z_0 \in \mathrm{Res}(H)$ *such that* $(H - z_0)^{-1} \in \mathcal{B}^n_A(\mathcal{H})$.

In practice it is useful to have a criteria characterizing $C^n_{\mathrm{loc}}(A)$-operators without reference to their resolvents. Moreover, Mourre theory requires the commutator $[A, H]$ to be defined as an operator, at least locally (in the sense of the spectrum of H). To this end we introduce a scale of Banach spaces.

Definition 4.13 *Let H be a self-adjoint operator on the Hilbert space $\mathcal{H}$, $\Lambda = (I + |H|)$, and $s \in \mathbb{R}$. We denote by $\mathcal{H}^s_H$ the Banach space obtained by completing* $\mathrm{Dom}(\Lambda^s)$ *equipped with the norm*

$$\|u\|_{H,s} = \|\Lambda^s u\|.$$

For $s \geq 0$ we have $\|u\|_{H,s} \geq \|u\|$ and the norm $\|\cdot\|_{H,s}$ is equivalent to the graph norm of the closed operator Λ^s. This implies that $\mathcal{H}^s_H = \mathrm{Dom}(\Lambda^s)$ and that Λ^s is an isometry from $\mathcal{H}^s_H$ onto $\mathcal{H}$. For $s \leq 0$ the map $u \mapsto \Lambda^{-s} u$ extends continuously to an isometry from $\mathcal{H}^{-s}_H$ onto $\mathcal{H}$ and

$$\mathcal{H}^s_H \times \mathcal{H}^{-s}_H \ni \langle u, v \rangle \mapsto (\Lambda^s u, \Lambda^{-s} v) \equiv (u, v), \tag{86}$$

describes the duality between $\mathcal{H}^{-s}_H$ and $\mathcal{H}^s_H$. We therefore obtain a scale of spaces

$$\mathcal{H}^{s'}_H \subset \mathcal{H}^s_H \subset \mathcal{H} = \mathcal{H}^0_H \subset \mathcal{H}^{-s}_H \subset \mathcal{H}^{-s'}_H,$$

for $0 \leq s \leq s'$, all embeddings being dense and continuous. We note in particular that for all $s \in \mathbb{R}$ one has $H \in \mathcal{B}(\mathcal{H}^s_H, \mathcal{H}^{s-1}_H)$ and $(H - z)^{-1} \in \mathcal{B}(\mathcal{H}^s_H, \mathcal{H}^{s+1}_H)$ for $z \in \mathrm{Res}(H)$.

Using the duality (86), we can associate to each continuous sesquilinear form $q\colon \mathcal{H}^s_H \times \mathcal{H}^s_H \to \mathbb{C}$ a unique operator $Q \in \mathcal{B}(\mathcal{H}^s_H, \mathcal{H}^{-s}_H)$ such that $q(u, v) = (u, Qv)$ for all $u, v \in \mathcal{H}^s_H$.

Lemma 4.14 *Let A and H be self-adjoint operators on the Hilbert space $\mathcal{H}$, and set $R(z) \equiv (H - z)^{-1}$. If $H \in C^n_{\mathrm{loc}}(A)$ then the following statements hold.*

(i) $\mathrm{Dom}(A) \cap \mathrm{Dom}(H)$ *is dense in* $\mathcal{H}$.

(ii) *For all* $z \in \mathrm{Res}(H)$ *and* $u, v \in \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$

$$(Au, Hv) - (Hu, Av) = -((H - z)^* u, [A, R(z)](H - z)v), \tag{87}$$

(iii) *There exists a constant c such that*

$$|(Au, Hu) - (Hu, Au)| \leq c\, \|u\|^2_{H,1},$$

for all $u \in \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$.

(iv) The quadratic form defined on $\mathrm{Dom}(A)\cap\mathrm{Dom}(H)$ *by the left hands side of Eq. (87) extends continuously to a bounded quadratic form on* $\mathscr{H}_H^1$.

Proof. (i) Lemma 4.12 shows that $H \in C^n_{\mathrm{loc}}(A)$ implies that $R(z_0) \in \mathscr{B}^n_A(\mathscr{H})$ for some $z_0 \in \mathrm{Res}(H)$. Since $\mathrm{Dom}(A)$ is dense in $\mathscr{H}$ and $R(z_0)^* = R(\overline{z}_0)$ is injective we may conclude that $R(z_0)\mathrm{Dom}(A)$ is dense. We finish the proof of assertion (i) by remarking that Lemma 4.2 implies that $R(z_0)\mathrm{Dom}(A) \subset \mathrm{Dom}(A)$ while the inclusion $R(z_0)\mathrm{Dom}(A) \subset \mathrm{Dom}(H)$ is evident.

(ii) For all $u, v \in \mathrm{Dom}(A)\cap\mathrm{Dom}(H)$ and $z \in \mathrm{Res}(H)$ we may write, with A_ε defined as in Lemma 4.6,

$$((H-z)^*u, [A_\varepsilon, R(z)](H-z)v) = ((H-z)^*u, A_\varepsilon v) - (A_\varepsilon^* u, (H-z)v) = (Hu, A_\varepsilon v) - (A_{-\varepsilon}u, Hv).$$

The proof of (ii) is obtained by taking the limit $\varepsilon \to 0$ and invoking Lemma 4.6.

(iii) is an immediate consequence of (ii) and the fact that $[A, R(z)]$ is bounded.

(iv) follows directly from (iii). □

Definition 4.15 *Let A and H be self-adjoint operators on the Hilbert space* $\mathscr{H}$ *such that* $\mathscr{D} = \mathrm{Dom}(A)\cap\mathrm{Dom}(H)$ *is dense in* $\mathscr{H}$. *If the sesquilinear form*

$$\mathscr{D}\times\mathscr{D} \ni \langle u, v\rangle \mapsto (Au, Hv) - (Hu, Av),$$

extends continuously to a bounded form on $\mathscr{H}_H^s$, *we denote by* $[A, H]$ *the operator associated with this extension, and we write* $[A, H] \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{-s})$.

Remark 4.1 If $[A, H] \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{-s})$ for some $s \geq 0$ then the operator $f(H)\mathrm{i}[A, H]f(H)$ is bounded on $\mathscr{H}$ for all $f \in C_0^\infty(\mathbb{R})$. In general however, we can not claim that it is self-adjoint.

Lemma 4.14 stipulates that if $H \in C^1_{\mathrm{loc}}(A)$ then $[A, H] \in \mathscr{B}(\mathscr{H}_H^1, \mathscr{H}_H^{-1})$. The converse is not true without an additional assumption. One possibility is given by the following result.

Lemma 4.16 *Let A and H be self-adjoint operators on the Hilbert space* $\mathscr{H}$ *and set* $R(z) = (H-z)^{-1}$. *The two following conditions are equivalent.*

(i) $H \in C^1_{\mathrm{loc}}(A)$.

(ii) $[A, H] \in \mathscr{B}(\mathscr{H}_H^1, \mathscr{H}_H^{-1})$ *and there exists* $z_0 \in \mathrm{Res}(H)$ *such that*

$$R(z_0)\mathrm{Dom}(A) \subset \mathrm{Dom}(A), \quad \textit{and} \quad R(\overline{z}_0)\mathrm{Dom}(A) \subset \mathrm{Dom}(A).$$

If one of these conditions is satisfied, then for each real measurable function f such that

$$\sup_{E\in\mathrm{Sp}(H)} (1+|E|)|f(E)| < \infty,$$

the operator $f(H)\mathrm{i}[A, H]f(H)$ *is bounded and self-adjoint on* $\mathscr{H}$. *Furthermore, if* $g \in C_0^\infty(\mathbb{R})$ *is such that* $g(E) = E$ *for all* $E \in \mathrm{supp}(f)$, *then*

$$f(H)\mathrm{i}[A, H]f(H) = f(H)\mathrm{ad}_A(g(H))f(H). \tag{88}$$

Proof. $(i) \Rightarrow (ii)$ is a direct consequence of the preceding remark and Lemmas 4.14, 4.12, and 4.2.

$(ii) \Rightarrow (i)$ By setting $C = [A, H]$ we may write

$$(Au, (H - z_0)v) - ((H - \overline{z}_0)u, Av) = (Au, Hv) - (Hu, Av) = (u, Cv),$$

for all $u, v \in \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$. Since $R(z_0)\mathrm{Dom}(A) \subset \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$ and $R(\overline{z}_0)\mathrm{Dom}(A) \subset \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$ by hypothesis, we also have

$$(AR(\overline{z}_0)u, (H - z_0)R(z_0)v) - ((H - \overline{z}_0)R(\overline{z}_0)u, AR(z_0)v) = (R(\overline{z}_0)u, CR(z_0)v),$$

that is,

$$(AR(\overline{z}_0)u, v) - (u, AR(z_0)v) = (R(\overline{z}_0)u, CR(z_0)v),$$

or also

$$(u, R(z_0)Av) - (Au, R(z_0)v) = (u, R(z_0)CR(z_0)v).$$

It follows from $C \in \mathscr{B}(\mathscr{H}^1_H, \mathscr{H}^{-1}_H)$ and $R(z_0) \in \mathscr{B}(\mathscr{H}, \mathscr{H}^1_H) \cap \mathscr{B}(\mathscr{H}^{-1}_H, \mathscr{H})$ that $R(z_0)CR(z_0) \in \mathscr{B}(\mathscr{H})$, and the last identity shows that $R(z_0) \in \mathscr{B}^1_A(\mathscr{H})$. The proof is finished by invoking Lemma 4.12.

To prove the final assertions of the lemma we note that $f(H) \in \mathscr{B}(\mathscr{H}, \mathscr{H}^1_H) \cap \mathscr{B}(\mathscr{H}^{-1}_H, \mathscr{H})$ since $\Lambda f(H)$ is bounded. This shows that $f(H)[A, H]f(H)$ is bounded. By Lemma 4.14 we have

$$(u, [A, H]v) = -((H - z)^* u, [A, R(z)](H - z)v),$$

for all $u, v \in \mathscr{H}^1_H$ and $z \in \mathrm{Res}(H)$. Thus

$$(f(H)u, [A, H]f(H)v) = -((H - z)^* f(H)u, [A, R(z)](H - z)f(H)v),$$

for all $u, v \in \mathscr{H}$. Since $Ef(E) = g(E)f(E)$ for all $E \in \mathbb{R}$ we may, without loss of generality, suppose that g is real and write the preceding relation as

$$(f(H)u, [A, H]f(H)v) = -(u, f(H)(g(H) - z)[A, R(z)](g(H) - z)f(H)v).$$

Lemma 4.6 allows us to write

$$f(H)(g(H) - z)[A, R(z)](g(H) - z)f(H)v = \lim_{\varepsilon \to 0} f(H)(g(H) - z)[A_\varepsilon, R(z)](g(H) - z)f(H)v,$$

and a simple calculation shows that $f(H)(g(H) - z)[A_\varepsilon, R(z)](g(H) - z)f(H)v = -[g(H), A_\varepsilon]v$. Since $g(H) \in \mathscr{B}_A(\mathscr{H})$ we may once again invoke Lemma 4.6 to obtain

$$\lim_{\varepsilon \to 0} [g(H), A_\varepsilon]v = [g(H), A]v,$$

and conclude that

$$(f(H)u, [A, H]f(H)v) = (f(H)u, [A, g(H)]f(H)v),$$

which proves (88). Finally, since ad_A is a $*$-derivation (Lemma 4.3), $\mathrm{ad}_A(g(H))$ is self-adjoint and so is $f(H)\mathrm{ad}_A(g(H))f(H)$. □

In practice it is often much easier to compute iterated commutators of A with H than $\mathrm{ad}_A^k((H-z)^{-1})$ and to verify the invariance of $\mathrm{Dom}(H)$ by the group $\mathrm{e}^{\mathrm{i}\theta A}$ than that of $\mathrm{Dom}(A)$ by the resolvent $(H-z)^{-1}$. The following results are therefore important in this cases.

Lemma 4.17 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$. The following statements hold if $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$ for all $\theta \in \mathbb{R}$.*

(i) $\mathrm{Dom}(A^\infty) \cap \mathscr{H}_H^s$ *is dense in* $\mathscr{H}_H^s$ *for all $s \in [-1,1]$.*

(ii) For all $s \in [0,1]$ and $\theta \in \mathbb{R}$ we have $\mathrm{e}^{\mathrm{i}\theta A}\mathscr{H}_H^s \subset \mathscr{H}_H^s$. The restriction of $\mathrm{e}^{\mathrm{i}\theta A}$ to $\mathscr{H}_H^s$ defines a strongly continuous, quasi-bounded group on $\mathscr{H}_H^s$. Its generator A_s is given by $\mathrm{Dom}(A_s) = \{u \in \mathscr{H}_H^s \,|\, u \in \mathrm{Dom}(A), Au \in \mathscr{H}_H^s\}$ *and $A_s u = Au$ for all $u \in \mathrm{Dom}(A_s)$.*

(iii) For all $s \in [0,1]$ and $\theta \in \mathbb{R}$ the operator $\mathrm{e}^{\mathrm{i}\theta A}$ extends continuously to $\mathscr{H}_H^{-s}$. This extension defines a strongly continuous, quasi-bounded group on $\mathscr{H}_H^{-s}$ which we denote again by $\mathrm{e}^{\mathrm{i}\theta A}$. Its generator A_{-s} is the closure of A in $\mathscr{H}_H^{-s}$.

(iv) For all $s \in [0,1]$, $u \in \mathscr{H}_H^{-s}$, $v \in \mathscr{H}_H^s$ and $\theta \in \mathbb{R}$, $(\mathrm{e}^{\mathrm{i}\theta A}u, \mathrm{e}^{\mathrm{i}\theta A}v) = (u,v)$. In particular $A_s^* = A_{-s}$.

Proof. To simplify our proof, we shall assume that $\mathscr{H}$ is separable and we refer the reader to proposition 3.2.5 of [ABG] for the general case. By hypothesis, the operator $\Lambda\mathrm{e}^{\mathrm{i}\theta A}\Lambda^{-1}$ is defined everywhere on $\mathscr{H}$. We easily verify that its graph is closed. This operator is thus bounded, which is equivalent to saying that $\mathrm{e}^{\mathrm{i}\theta A}$ is bounded on $\mathscr{H}_H^1$. We thus have $\mathrm{e}^{\mathrm{i}\theta A} \in \mathscr{B}(\mathscr{H}_H^1) \cap \mathscr{B}(\mathscr{H}_H^0)$ from which we deduce $\mathrm{e}^{\mathrm{i}\theta A} \in \mathscr{B}(\mathscr{H}_H^s)$ for all $s \in [0,1]$ by interpolation.

Since $\mathscr{H}$ is separable it has a dense countable subset $\mathscr{D}_0$. The sets $\mathscr{D}_+ \equiv \{\Lambda^{-s}v/\|v\| \,|\, v \in \mathscr{D}_0, v \neq 0\} \subset \mathscr{H}$ and $\mathscr{D}_- \equiv \{v/\|\Lambda^{-s}v\| \,|\, v \in \mathscr{D}_0, v \neq 0\} \subset \mathscr{H}$ are countable and dense in the unit spheres of $\mathscr{H}_H^{\pm s}$. For all $\theta \in \mathbb{R}$ we thus have

$$\|\mathrm{e}^{\mathrm{i}\theta A}\|_{\mathscr{B}(\mathscr{H}_H^s)} = \sup_{\langle u,v\rangle \in \mathscr{D}_- \times \mathscr{D}_+} |(u, \mathrm{e}^{\mathrm{i}\theta A}v)|.$$

Since $\mathscr{D}_- \times \mathscr{D}_+$ is countable and $\theta \mapsto |(u, \mathrm{e}^{\mathrm{i}\theta A}v)|$ is continuous and thus measurable for all $\langle u,v\rangle \in \mathscr{D}_- \times D_+ \subset \mathscr{H} \times \mathscr{H}$, the functions $f_\pm(\theta) = \log\|\mathrm{e}^{\pm\mathrm{i}\theta A}\|_{\mathscr{B}(\mathscr{H}_H^s)}$ are measurable. They are sub-additive ($f_\pm(\theta+\theta') \le f_\pm(\theta) + f_\pm(\theta')$) and thus bounded on all compact intervals (see, for example, Theorem 7.4.1 in [HP]). We easily conclude that for all $\delta > 0$, $\theta \ge 0$,

$$f_\pm(\theta) \le \theta\frac{|f_\pm(\delta)|}{\delta} + \sup_{\vartheta \in [0,\delta]} f_\pm(\vartheta),$$

which shows that the group $\mathrm{e}^{\mathrm{i}\theta A}$ is quasi-bounded on $\mathscr{H}_H^1$,

$$\|\Lambda^s\mathrm{e}^{\mathrm{i}\theta A}\Lambda^{-s}\| = \|\mathrm{e}^{\mathrm{i}\theta A}\|_{\mathscr{B}(\mathscr{H}^s)} \le M\mathrm{e}^{\omega|\theta|}, \tag{89}$$

for some constants M and ω and all $\theta \in \mathbb{R}$. For $u \in \mathcal{H}$ and $\varepsilon > 0$ we set

$$u_\varepsilon \equiv \mathrm{e}^{-\varepsilon^2 A^2/4} u = \pi^{-1/2} \int_{-\infty}^{\infty} \mathrm{e}^{-\vartheta^2} \, \mathrm{e}^{\mathrm{i}\varepsilon\vartheta A} u \, \mathrm{d}\vartheta.$$

We easily show that, for all $u \in \mathcal{H}$, $\lim_{\varepsilon\to 0} \|u_\varepsilon - u\| = 0$. Furthermore, the bound (89) implies $\|u_\varepsilon\|_{H,s} \le c\,\|u\|_{H,s}$ for a constant c and $\varepsilon \in]0,1]$. Since $\mathcal{H}$ is dense in $\mathcal{H}_H^{-s}$ we may conclude that u_ε converges to u in the weak topology of $\mathcal{H}_H^s$. It follows that $\mathcal{D} \equiv \{u_\varepsilon \,|\, u \in \mathcal{H}_H^s, \varepsilon > 0\}$ is dense in $\mathcal{H}$ and thus in $\mathcal{H}_H^s$. The identity

$$(\mathrm{e}^{\mathrm{i}\theta A} - I)\, u_\varepsilon = \pi^{-1/2} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-(\vartheta-\theta/\varepsilon)^2} - \mathrm{e}^{-\vartheta^2} \right) \mathrm{e}^{\mathrm{i}\varepsilon\vartheta A} u \, \mathrm{d}\vartheta,$$

and the bound (89) lead to

$$\|(\mathrm{e}^{\mathrm{i}\theta A} - I)\, u_\varepsilon\|_{H,s} \le \pi^{-1/2} \int_{-\infty}^{\infty} \left| \mathrm{e}^{-(\vartheta-\theta/\varepsilon)^2} - \mathrm{e}^{-\vartheta^2} \right| M \mathrm{e}^{\varepsilon|\vartheta|\omega} \|u\|_{H,s} \, \mathrm{d}\vartheta.$$

We deduce that $\lim_{\theta\to 0} \|(\mathrm{e}^{\mathrm{i}\theta A} - I)\, u\|_{H,s} = 0$ for all $u \in \mathcal{D}$. The bound (89) and the density of $\mathcal{D}$ allow us to conclude that $\theta \mapsto \mathrm{e}^{\mathrm{i}\theta A}$ is strongly continuous on $\mathcal{H}_H^s$. Let A_s be the generator of this group. If $u \in \mathrm{Dom}(A_s)$ then

$$\lim_{\theta\to 0} \left\| \frac{\mathrm{e}^{\mathrm{i}\theta A} u - u}{\mathrm{i}\theta} - A_s u \right\|_{H,s} = 0.$$

We conclude that $u \in \mathrm{Dom}(A)$ and that $Au = A_s u \in \mathcal{H}_H^s$. Conversely, if $u \in \mathrm{Dom}(A) \cap \mathcal{H}_H^s$ and $v = Au \in \mathcal{H}_H^s$ then the identity

$$\frac{\mathrm{e}^{\mathrm{i}\theta A} u - u}{\mathrm{i}\theta} - v = \int_0^1 \left(\mathrm{e}^{\mathrm{i}t\theta A} - I \right) v \, \mathrm{d}t,$$

the bound (89), and the continuity of $t \mapsto \mathrm{e}^{\mathrm{i}t\theta A} v$ in $\mathcal{H}_H^s$ allow us to conclude that $u \in \mathrm{Dom}(A_s)$. Finally we note that $\mathcal{D} \subset \mathrm{Dom}(A^\infty) \cap \mathcal{H}_H^s$, which finishes the proof for assertions (i) and (ii) for $s \in [0,1]$.

By duality $(T^\theta u, v) \equiv (u, \mathrm{e}^{\mathrm{i}\theta A} v)$ defines a strongly continuous, quasi-bounded group on $\mathcal{H}_H^{-s}$. Furthermore, $T^\theta = \mathrm{e}^{-\mathrm{i}\theta A}$ on the dense subspace $\mathcal{H} \subset \mathcal{H}_H^{-s}$. T^θ is thus the unique continuous extension of $\mathrm{e}^{\mathrm{i}\theta A}$ to $\mathcal{H}_H^{-s}$. Since $\mathrm{Dom}(A)$ is dense in $\mathcal{H}$ it is also dense in $\mathcal{H}_H^{-s}$. Furthermore it is invariant by T^θ. It is thus a core for the generator A_s of T^θ (see Theorem X.49 in [RS2]). The same argument applies to $\mathrm{Dom}(A^\infty)$. The assertions (ii) for $s \in [-1,0]$ and (iii) are proven. Assertion (iv) is an immediate consequence of the duality. □

With a small abuse of notation, we shall denote by A the generator A_s when the space on which it acts is clearly determined by the context. Similarly, A_ε will denote the element of $\mathcal{B}(\mathcal{H}_H^s)$ corresponding to the restriction (for $s \ge 0$) or the continuous extension (for $s \le 0$) of the operator $(\mathrm{i}\varepsilon)^{-1}(\mathrm{e}^{\mathrm{i}\varepsilon A} - I)$ on $\mathcal{H}_H^s$.

Under the hypotheses of Lemma 4.17, if $B \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ with $s, s' \in [-1,1]$, then one has $B^* \in \mathscr{B}(\mathscr{H}_H^{-s'}, \mathscr{H}_H^{-s})$ and

$$(Au, Bv) - (B^* u, Av),$$

defines a quadratic form on $\mathrm{Dom}(A_{-s'}) \times \mathrm{Dom}(A_s)$. If there exists a constant c such that, for all $\langle u, v\rangle \in \mathrm{Dom}(A_{-s'}) \times \mathrm{Dom}(A_s)$,

$$|(Au, Bv) - (B^* u, Av)| \leq c \, \|u\|_{H,-s'} \, \|v\|_{H,s},$$

then there exists an operator $C \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ such that

$$(Au, Bv) - (B^* u, Av) = (u, Cv).$$

In this case we shall write $C = [A, B]$ and, when this construction can be iterated, we define $\mathrm{ad}_A^k(B) \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ as before.

Definition 4.18 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$ such that, for all $\theta \in \mathbb{R}$, $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$. For all $n \in \mathbb{N}$, we denote*

$$\mathscr{B}_A^n(\mathscr{H}_H^s, \mathscr{H}_H^{s'}) \equiv \{B \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'}) \,|\, \mathrm{ad}_A^k(B) \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'}), k = 0, \ldots, n\}.$$

In particular $\mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'}) = \mathscr{B}_A^0(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ and $\mathscr{B}_A(\mathscr{H}_H^s, \mathscr{H}_H^{s'}) = \mathscr{B}_A^1(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$.

Lemma 4.19 *Let A and H be self-adjoint operators on $\mathscr{H}$ such that $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$ for all $\theta \in \mathbb{R}$.*

(i) $B \in \mathscr{B}_A^n(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ if and only if $\sup_{\varepsilon \in \mathbb{R}^*} \|\mathrm{ad}_{A_\varepsilon}^n(B)\|_{\mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'})} < \infty$ and in this case

$$\mathrm{ad}_A^n(B)v = \lim_{\varepsilon \to 0} \mathrm{ad}_{A_\varepsilon}^n(B)v,$$

in $\mathscr{H}_H^{s'}$ for all $v \in \mathscr{H}_H^s$.

(ii) $B \in \mathscr{B}_A(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ if and only if $B^* \in \mathscr{B}_A(\mathscr{H}_H^{-s'}, \mathscr{H}_H^{-s})$. Furthermore

$$\mathrm{ad}_A(B^*) = \mathrm{ad}_A(B)^*.$$

(iii) If $B \in \mathscr{B}_A(\mathscr{H}_H^{s'}, \mathscr{H}_H^{s''})$ and $C \in \mathscr{B}_A(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$ then $BC \in \mathscr{B}_A(\mathscr{H}_H^s, \mathscr{H}_H^{s''})$ and

$$\mathrm{ad}_A(BC) = \mathrm{ad}_A(B)C + B\mathrm{ad}_A(C).$$

Proof. The proof of Lemma 4.6 is easily adapted to prove assertion (i).

(ii) is a direct consequence of the identity

$$(Au, Bv) - (B^* u, Av) = -\overline{(Av, B^* u) - (Bv, Au)}.$$

(iii) For $\langle u, v\rangle \in \mathrm{Dom}(A_{-s''}) \times \mathrm{Dom}(A_s)$ we have

$$\begin{aligned}(Au, BCv) - (C^* B^* u, Av) &= \lim_{\varepsilon\to 0}(A_{-\varepsilon} u, BCv) - (C^* B^* u, A_\varepsilon v)\\ &= \lim_{\varepsilon\to 0}(u, A_\varepsilon BCv - BCA_\varepsilon v)\\ &= \lim_{\varepsilon\to 0}(u, [A_\varepsilon, B]Cv + B[A_\varepsilon, C]v)\\ &= -\lim_{\varepsilon\to 0}([A_{-\varepsilon}, B^*]u, Cv) + \lim_{\varepsilon\to 0}(B^* u, [A_\varepsilon, C]v).\end{aligned}$$

The assertions (i) and (ii) allows us to conclude that

$$\lim_{\varepsilon\to 0}[A_{-\varepsilon}, B^*]u = [A, B^*]u = -[A, B]^* u,$$

in $\mathscr{H}_H^{-s'}$ and that

$$\lim_{\varepsilon\to 0}[A_\varepsilon, C]v = [A, C]v,$$

in $\mathscr{H}_H^{s'}$. It is then easy to finish the proof. □

Definition 4.20 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$ such that, for all $\theta \in \mathbb{R}$, $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$. An operator $B \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$, with $s, s' \in [-1, 1]$, is of class $C^n(A; H; s, s')$ if, for all $v \in \mathscr{H}_H^s$ the function*

$$\begin{array}{ccc}\mathbb{R} & \to & \mathscr{H}_H^{s'}\\ \theta & \mapsto & \mathrm{e}^{\mathrm{i}\theta A} B \mathrm{e}^{-\mathrm{i}\theta A} v,\end{array}$$

is of class C^n.

Lemma 4.21 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$ such that, for all $\theta \in \mathbb{R}$, $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$. For an operator $B \in \mathscr{B}(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$, the following are equivalent*

(i) $B \in C^n(A; H; s, s')$ and $B^* \in C^n(A; H; -s', -s)$.

(ii) $B \in \mathscr{B}_A^n(\mathscr{H}_H^s, \mathscr{H}_H^{s'})$.

If one of these statements holds, then

$$\frac{\mathrm{d}^k}{\mathrm{d}\theta^k}\mathrm{e}^{\mathrm{i}\theta A} B \mathrm{e}^{-\mathrm{i}\theta A} v = \mathrm{e}^{\mathrm{i}\theta A}\mathrm{ad}_A^k(B)\mathrm{e}^{-\mathrm{i}\theta A} v,$$

for $k = 1, \ldots, n$ and $v \in \mathscr{H}_H^s$.

Proof. The strategy is identical to that of the proof of Lemma 4.5 □

Theorem 4.22 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$ such that, for all $\theta \in \mathbb{R}$, $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$.*

(i) $H \in C^1_{\mathrm{loc}}(A)$ *if and only if* $H \in \mathscr{B}_A(\mathscr{H}^1_H, \mathscr{H}^{-1}_H)$.

(ii) *If* $H \in \mathscr{B}^n_A(\mathscr{H}^1_H, \mathscr{H})$ *then* $H \in C^n_{\mathrm{loc}}(A)$.

Proof. (i) By combining Lemmas 4.6 and 4.19, it suffices to show that for $z \in \mathrm{Res}(H)$,

$$\sup_{\varepsilon\in\mathbb{R}^*} \|[A_\varepsilon, R(z)]\| < \infty \Longleftrightarrow \sup_{\varepsilon\in\mathbb{R}^*} \|[A_\varepsilon, H]\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H}^{-1}_H)} < \infty.$$

For all $s \in \mathbb{R}$, $R(z)$ is an isomorphism of $\mathscr{H}^s_H$ into $\mathscr{H}^{s+1}_H$, with inverse $H - z$. For $u \in \mathscr{H}^1_H$ the identity

$$[A_\varepsilon, H]u = [A_\varepsilon, H - z]u = A_\varepsilon(H - z)u - (H - z)A_\varepsilon u = (H - z)\,[R(z)A_\varepsilon - A_\varepsilon R(z)]\,(H - z)u,$$

implies

$$\|[A_\varepsilon, H]\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H}^{-1}_H)} \le \|H - z\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H})}\|[A_\varepsilon, R(z)]\|\,\|H - z\|_{\mathscr{B}(\mathscr{H},\mathscr{H}^{-1}_H)},$$

and thus $\sup_{\varepsilon\in\mathbb{R}^*}\|[A_\varepsilon, R(z)]\| < \infty \Rightarrow \sup_{\varepsilon\in\mathbb{R}^*}\|[A_\varepsilon, H]\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H}^{-1}_H)} < \infty$. Conversely, we have, for $u \in \mathscr{H}$,

$$[A_\varepsilon, R(z)]u = R(z)\,[HA_\varepsilon - A_\varepsilon H]\,R(z)u,$$

which implies

$$\|[A_\varepsilon, R(z)]\| \le \|R(z)\|_{\mathscr{B}(\mathscr{H}^{-1}_H,\mathscr{H})}\|[A_\varepsilon, H]\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H}^{-1}_H)}\|R(z)\|_{\mathscr{B}(\mathscr{H},\mathscr{H}^1_H)},$$

and thus $\sup_{\varepsilon\in\mathbb{R}^*}\|[A_\varepsilon, H]\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H}^{-1}_H)} < \infty \Rightarrow \sup_{\varepsilon\in\mathbb{R}^*}\|[A_\varepsilon, R(z)]\| < \infty$.
(ii) Let $z \in \mathrm{Res}(H)$ and $R = (H - z)^{-1}$. We easily show, by induction on k, that

$$\mathrm{ad}^k_{A_\varepsilon}(R) = \sum_{l=1}^{k} \sum_{k_1+\cdots+k_l=k} C^{(l)}_{k_1\ldots k_l} R\,\mathrm{ad}^{k_1}_{A_\varepsilon}(H)R\,\mathrm{ad}^{k_2}_{A_\varepsilon}(H)R\cdots\mathrm{ad}^{k_l}_{A_\varepsilon}(H)R,$$

where the $C^{(l)}_{k_1\ldots k_l}$ are numerical coefficients. Since

$$\|\mathrm{ad}^k_{A_\varepsilon}(H)R\| \le \|\mathrm{ad}^k_{A_\varepsilon}(H)\|_{\mathscr{B}(\mathscr{H}^1_H,\mathscr{H})}\,\|R\|_{\mathscr{B}(\mathscr{H},\mathscr{H}^1_H)},$$

Lemma 4.19 implies that if $H \in \mathscr{B}^n_A(\mathscr{H}^1_H, \mathscr{H})$ we have

$$\sup_{\varepsilon\in\mathbb{R}^*} \|\mathrm{ad}^n_{A_\varepsilon}(R)\| < \infty,$$

and Lemma 4.6 allows us to conclude that $R \in C^n(A)$. Finally, Lemma 4.12 shows that $H \in C^n_{\mathrm{loc}}(A)$. $\square$

4.2 The Mourre estimate

The following definition is due to Mourre [M1].

Definition 4.23 *Let H and A be self-adjoint operators on the Hilbert space $\mathcal{H}$.*

(i) H satisfies a Mourre estimate at $E \in \mathbb{R}$ with the conjugate operator A if there exists $\theta > 0$, a function $g \in C_0^\infty(\mathbb{R})$ and a compact operator K such that $0 \le g \le 1$, $g(E) = 1$ and

$$g(H)\mathrm{i}[H, A]g(H) \ge \theta g(H)^2 + K. \tag{90}$$

(ii) Let $O \subset \mathbb{R}$ be open. H satisfies a Mourre estimate on O with the conjugate operator A if, for all $E \in O$, H satisfies a Mourre estimate with the conjugate operator A at E.

(iii) If it is possible to take $K = 0$ in (90), we say that H satisfies a strict Mourre estimate at E (respectively on O) with the conjugate operator A.

The following lemma shows that the set of E at which H satisfies a (strict) Mourre estimate with the conjugate operator A is open.

Lemma 4.24 *If H satisfies a (strict) Mourre estimate at $E \in \mathbb{R}$, there exists an open interval $\Delta \ni E$ such that (90) is satisfied with $g = 1_\Delta$, the indicator function of Δ (and $K = 0$).*

Proof. By hypothesis, there exists $\theta > 0$, $g \in C_0^\infty(\mathbb{R})$ such that $0 \le g \le 1$, $g(E) = 1$, as well as a compact operator K satisfying (90). There thus exists $\delta > 0$ such that $\Delta \equiv]E-\delta, E+\delta[\subset g^{-1}(]1/2, 1])$. It follows that $0 \le h \equiv 1_\Delta/g \le 2$ and in particular that $h(H)$ is bounded. By multiplying (90) on both sides by $h(H)$ we obtain

$$1_\Delta(H)\mathrm{i}[H, A]1_\Delta(H) \ge \theta 1_\Delta(H) + K',$$

where $K' = h(H)Kh(H)$ is compact (and vanishes if $K = 0$). □

The first consequences of the Mourre estimate concern the singular spectrum of H (see [M1]).

Theorem 4.25 *We suppose that a self-adjoint operator H on the Hilbert space $\mathcal{H}$ satisfies a Mourre estimate on the open set $O \subset \mathbb{R}$ with the conjugate operator A.*

(i) If $H \in C^1_{\mathrm{loc}}(A)$ and $I \subset O$ is compact then $\mathrm{Sp}_{\mathrm{pp}}(H) \cap I$ is finite. This set is empty if the Mourre estimate is strict on I.

(ii) If $H \in C^2_{\mathrm{loc}}(A)$ then $\mathrm{Sp}_{\mathrm{sc}}(H) \cap O$ is empty.

Proof. We essentially follow the proof in [M1].

(i) For all $E \in O$ we denote by $\Delta_E \ni E$ the interval described in Lemma 4.24. We thus have the Mourre estimate

$$1_{\Delta_E}(H)\mathrm{i}[H, A]1_{\Delta_E}(H) \ge \theta_E 1_{\Delta_E}(H) + K_E, \tag{91}$$

for a constant $\theta_E > 0$ and a compact operator K_E. We fix $f_E \in C_0^\infty(\mathbb{R})$ such that $f_E(x)1_{\Delta_E}(x) = x$ for all $x \in \Delta_E$.

If $E_0 \in \mathrm{Sp_{pp}}(H) \cap \Delta_E$, $Hu = E_0 u$ and $\|u\| = 1$ we have $1_{\Delta_E}(H)u = u$ and $f_E(H)u = E_0 u$. Since $H \in C^1_{\mathrm{loc}}(A)$, $[A, f_E(H)]$ is bounded and Lemmas 4.6 and 4.5 imply

$$(u, \mathrm{i}[f_E(H), A]u) = \lim_{\varepsilon\to 0}(u, \mathrm{i}[f_E(H), A_\varepsilon]u) = \mathrm{i}E_0 \lim_{\varepsilon\to 0}(u, A_\varepsilon u) - (A_\varepsilon^* u, u) = 0.$$

Identity (88) and the Mourre estimate (91) allow us to write

$$0 = (u, \mathrm{i}[f_E(H), A]u) = (u, 1_{\Delta_E}(H)\mathrm{i}[H, A]1_{\Delta_E}(H)u) \geq \theta_E + (u, K_E u),$$

and thus

$$0 < \theta_E \leq |(u, K_E u)|. \tag{92}$$

Suppose now that $\mathrm{Sp_{pp}}(H) \cap \Delta_E$ is infinite. There thus exists a sequence $E_n \in \mathrm{Sp_{pp}}(H) \cap \Delta_E$ and a corresponding orthonormal sequence u_n of eigenvectors. It follows that $\mathrm{w}-\lim_n u_n = 0$ and, since K_E is compact, $\lim_n \|K_E u_n\| = 0$. We deduce that

$$0 < \theta_E \leq |(u_n, K_E u_n)| \leq \|K_E u_n\| \to 0 \quad (n \to \infty),$$

a contradiction which shows that $\mathrm{Sp_{pp}}(H) \cap \Delta_E$ is finite.

We have shown that every $E \in O$ has an open neighborhood Δ_E such that $\Delta_E \cap \mathrm{Sp_{pp}}(H)$ is finite. If $I \subset O$ is compact there exists a finite set $\mathscr{E} \subset O$ such that

$$I \subset \bigcup_{E\in\mathscr{E}} \Delta_E,$$

and we conclude that $\mathrm{Sp_{pp}}(H) \cap I$ is finite.

If the Mourre estimate is strict on I then $K_E = 0$ for all $E \in I$ and (92) leads to a contradiction which forces us to conclude that $\Delta_E \cap \mathrm{Sp_{pp}}(H)$ is empty and in particular that $E \notin \mathrm{Sp_{pp}}(H)$.

(ii) Let $E \in O \setminus \mathrm{Sp_{pp}}(H)$. Assertion (i) implies that there exists $\delta > 0$ such that $]E-\delta, E+\delta[\subset O \setminus \mathrm{Sp_{pp}}(H)$. By denoting $P_\varepsilon \equiv 1_{]E-\varepsilon, E+\varepsilon[}(H)$ we thus have $\mathrm{w}-\lim_{\varepsilon\to 0} P_\varepsilon = 0$ and consequently $\lim_{\varepsilon\to 0} \|P_\varepsilon K P_\varepsilon\| = 0$. We deduce that if ε is small enough then $\|P_\varepsilon K P_\varepsilon\| \leq \theta/2$ and

$$P_\varepsilon \mathrm{i}[H, A]P_\varepsilon \geq \theta P_\varepsilon + P_\varepsilon K P_\varepsilon \geq \frac{\theta}{2} P_\varepsilon \geq 0.$$

In the following, we fix such an ε, we set $I \equiv]E-\varepsilon/2, E+\varepsilon/2[$ and we denote

$$\Omega_\gamma \equiv \{\langle z, \mu\rangle \in \mathbb{C}\setminus\mathbb{R} \times \mathbb{R} \,|\, \mathrm{Re}\, z \in I, \mathrm{sign}\,(\mu) = \mathrm{sign}\,(\mathrm{Im}\, z), 0 < |\mu| < \gamma\},$$

where the constant $\gamma > 0$ will be fixed later. We also choose a function $g \in C_0^\infty(]E-\varepsilon, E+\varepsilon[)$ such that $0 \leq g \leq 1$ and $g = 1$ on $[E - 3\epsilon/4, E + 3\epsilon/4]$. We thus have

$$Q \equiv g(H)\mathrm{i}[H, A]g(H) \geq \frac{\theta}{2} g(H)^2 \geq 0. \tag{93}$$

Since $H \in C^1_{\mathrm{loc}}(A)$, Lemma 4.16 implies that Q is a bounded self-adjoint operator. The operator $K_\mu \equiv H - \mathrm{i}\mu Q$ is thus closed on $\mathrm{Dom}(H)$. For $\langle z, \mu\rangle \in \Omega_\gamma$ we have

$$\|u\|\,\|(K_\mu - z)u\| \geq |(u,(K_\mu - z)u)| \geq |\mathrm{Im}(u,(H - \mathrm{i}\mu Q - z)u)| \geq |\mathrm{Im}\, z|\,\|u\|^2,$$

for all $u \in \mathrm{Dom}(H)$. We deduce

$$\|u\| \leq |\mathrm{Im}\, z|^{-1}\|(K_\mu - z)u\|, \tag{94}$$

so that $\mathrm{Ker}\,(K_\mu - z) = \{0\}$. We show that this inequality also implies that $\mathrm{Ran}\,(K_\mu - z)$ is closed. If $v_n = (K_\mu - z)u_n$ for a sequence $u_n \in \mathrm{Dom}(H)$ and if $\lim_n v_n = v$ then (94) implies that $\|u_n - u_m\| \leq \|v_n - v_m\|/|\mathrm{Im(z)}|$ which shows that u_n is Cauchy. Let $u = \lim_n u_n$. Since $K_\mu - z$ is closed, it follows that $u \in \mathrm{Dom}(K_\mu) = \mathrm{Dom}(H)$, $v = (K_\mu - z)u$ and thus that $v \in \mathrm{Ran}\,(K_\mu - z)$.
If $u \in \mathrm{Ran}\,(K_\mu - z)^\perp$ then, for all $v \in \mathrm{Dom}(H)$, we have

$$(u,(K_\mu - z)v) = (u, Hv) - (u,(z + \mathrm{i}\mu Q)v) = 0,$$

and thus

$$|(u, Hv)| \leq (|z| + |\mu|\,\|Q\|)\,\|u\|\,\|v\|.$$

We deduce that $u \in \mathrm{Dom}(H)$ and that

$$((H - \overline{z} + \mathrm{i}\mu Q)u, v) = 0,$$

for all $v \in \mathrm{Dom}(H)$. It follows that $u \in \mathrm{Ker}\,(K_{-\mu} - \overline{z})$ and since $\langle \overline{z}, -\mu\rangle \in \Omega_\gamma$ it follows that $u = 0$. We have thus shown that $\mathrm{Ran}\,(K_\mu - z) = \mathscr{H}$. The inverse operator

$$G_\mu(z) \equiv (K_\mu - z)^{-1},$$

being closed with domain $\mathscr{H}$ is bounded. Furthermore, we clearly have $G_\mu(z)^* = G_{-\mu}(\overline{z})$.
The Mourre estimate (93) further gives

$$\begin{aligned} G_\mu(z)^* g(H)^2 G_\mu(z) &\leq \frac{2}{\theta} G_\mu(z)^* Q G_\mu(z) \\ &\leq \frac{2}{\theta\mu} G_\mu(z)^* (\mathrm{Im}\, z + \mu Q) G_\mu(z) \\ &= \frac{\mathrm{i}}{\theta\mu}(G_\mu(z)^* - G_\mu(z)), \end{aligned} \tag{95}$$

from which we conclude that $\|g(H)G_\mu(z)\|^2 \leq 2\|G_\mu(z)\|/\theta|\mu|$. Using the second resolvent identity $G_\mu(z) = G_0(z)(I + \mathrm{i}\mu Q G_\mu(z))$ we can write

$$G_\mu(z)^* G_\mu(z) = G_\mu(z)^* g(H)^2 G_\mu(z) + G_\mu(z)^*(1 - g(H)^2) G_0(z)(I + \mathrm{i}\mu Q G_\mu(z)).$$

Since $G_0(z) = (H - z)^{-1}$ and $\mathrm{dist}(I, \mathrm{supp}(1 - g^2)) \geq \epsilon/4$, the functional calculus yields the estimate $\|(1 - g(H)^2)G_0(z)\| \leq 4/\epsilon$ for $\mathrm{Re}\, z \in I$ and we obtain

$$\|G_\mu(z)\|^2 \leq \frac{2}{\theta|\mu|}\|G_\mu(z)\| + \frac{4}{\epsilon}(1 + |\mu|\|Q\|\,\|G_\mu(z)\|)\|G_\mu(z)\|.$$

Rewriting the last inequality as

$$\left(1-\frac{4\|Q\||\mu|}{\epsilon}\right)\|\mu G_\mu(z)\| \le \frac{2}{\theta}+\frac{4|\mu|}{\epsilon},$$

it is easy to conclude that

$$\sup_{\langle z,\mu\rangle\in\Omega_\gamma}\|\mu G_\mu(z)\| \le \frac{2}{\theta}\frac{\epsilon+2\theta\gamma}{\epsilon-4\|Q\|\gamma}<\infty, \tag{96}$$

provided we impose $\gamma<\epsilon/4\|Q\|$.

We shall denote $T\equiv|A+\mathrm{i}|^{-1}$, $\Lambda\equiv(1+|H|)$, and we shall use the notation introduced in Definition 4.13 in what follows.

Multiplying the inequality (95) on both sides with T gives

$$\|g(H)G_\mu(z)T\|^2 \le \frac{2}{\theta|\mu|}\|TG_\mu(z)T\|.$$

Since $g(H)\Lambda^2 g(H)\le Cg(H)^2$, it follows that there exists a constant C_1 such that

$$\|g(H)G_\mu(z)T\|_{\mathscr{B}(\mathscr{H},\mathscr{H}_H^1)} \le C_1|\mu|^{-1/2}\|TG_\mu(z)T\|^{1/2}, \tag{97}$$

for all $\langle z,\mu\rangle\in\Omega_\gamma$.

Using again the second resolvent equation, we can write

$$\|\Lambda(1-g(H))G_\mu(z)\| \le \|\Lambda(1-g(H))G_0(z)\|\,(I+\|Q\|\,\|\mu G_\mu(z)\|),$$

and the functional calculus and inequality (96) yield

$$C_2\equiv\sup_{\langle z,\mu\rangle\in\Omega_\gamma}\|(I-g(H))G_\mu(z)\|_{\mathscr{B}(\mathscr{H},\mathscr{H}_H^1)}<\infty. \tag{98}$$

By combining this last estimate and (97) we obtain

$$\begin{aligned}\|G_\mu(z)T\|_{\mathscr{B}(\mathscr{H},\mathscr{H}_H^1)} &\le \|g(H)G_\mu(z)T\|_{\mathscr{B}(\mathscr{H},\mathscr{H}_H^1)}+\|(1-g(H))G_\mu(z)\|_{\mathscr{B}(\mathscr{H},\mathscr{H}_H^1)}\,\|T\|\\ &\le C_1|\mu|^{-1/2}\|TG_\mu(z)T\|^{1/2}+C_2. \end{aligned} \tag{99}$$

Since $\operatorname{Ran} G_\mu(z)=\operatorname{Dom}(H)=\mathscr{H}_H^1$, and $[H,A]\in\mathscr{B}(\mathscr{H}_H^1,\mathscr{H}_H^{-1})$ by Lemma 4.16, the identity

$$Q=\mathrm{i}[H,A]-g(H)\mathrm{i}[H,A](1-g(H))-(1-g(H))\mathrm{i}[H,A]g(H)-(1-g(H))\mathrm{i}[H,A](I-g(H)),$$

may be substituted into

$$\frac{\mathrm{d}}{\mathrm{d}\mu}TG_\mu(z)T=\mathrm{i}TG_\mu(z)QG_\mu(z)T,$$

to obtain, using (97) and (98),

$$\left\| \frac{\mathrm{d}}{\mathrm{d}\mu} TG_\mu(z)T \right\| \le \|TG_\mu(z)[H,A]G_\mu(z)T\| + C_2 \|[H,A]\|_{\mathscr{B}(\mathscr{H}_H^1,\mathscr{H}_H^{-1})} \left(C_2 + 2C_1 |\mu|^{-1/2} \|TG_\mu(z)T\|^{1/2}\right). \tag{100}$$

To estimate the first term on the right hand side of this inequality, we decompose

$$[H,A] = [K_\mu - z, A] + \mathrm{i}\mu[Q,A].$$

Let $f \in C_0^\infty(\mathbb{R})$ be such that $f(x)g(x) = xg(x)$. By invoking Lemma 4.16 we remark that

$$\begin{aligned}[Q,A] =& \mathrm{i}[A, g(H)[A,f(H)]g(H)] \\ =& \mathrm{i}g(H)[A,f(H)][A,g(H)] + \mathrm{i}[A,g(H)][A,f(H)]g(H) + \mathrm{i}g(H)[A,[A,f(H)]]g(H),\end{aligned}$$

and since $H \in C^2_{\mathrm{loc}}(A)$, we can conclude that $[Q,A]$ is bounded. The estimate (99) gives us

$$\|TG_\mu(z)\mathrm{i}\mu[Q,A]G_\mu(z)T\| \le \|[Q,A]\| \, (C_1 \|TG_\mu(z)T\|^{1/2} + C_2|\mu|^{1/2})^2. \tag{101}$$

Also, the identity

$$G_\mu(z)[K_\mu - z, A]G_\mu(z) = [A, G_\mu(z)],$$

and the estimate (99) allows us to write

$$\begin{aligned}\|TG_\mu(z)[K_\mu - z, A]G_\mu(z)T\| &= \|T[A, G_\mu(z)]T\| \\ &\le \|G_\mu(z)T\| + \|TG_\mu(z)\| \\ &\le 2(C_1|\mu|^{-1/2}\|TG_\mu(z)T\|^{1/2} + C_2).\end{aligned} \tag{102}$$

By combining (101) and (102) in (100) we obtain, after taking into account (96), the following differential inequality.

$$\left\| \frac{\mathrm{d}}{\mathrm{d}\mu} TG_\mu(z)T \right\| \le a + b\|TG_\mu(z)T\| + c\frac{\|TG_\mu(z)T\|^{1/2}}{|\mu|^{1/2}},$$

valid for all $\langle z,\mu\rangle \in \Omega_\gamma$ and where a, b, c are positive constants. Setting $\phi(\mu) = \|TG_\mu(z)T\|$ we can write, for $0 < \mu < \mu_0 < \gamma$,

$$\begin{aligned}\phi(\mu) &\le \phi(\mu_0) + \int_\mu^{\mu_0} (a + b\phi(\nu) + c\nu^{-1/2}\phi(\nu)^{1/2})\,\mathrm{d}\nu \\ &\le \Phi(\mu) \equiv (\phi(\mu_0) + a\mu_0) + \int_\mu^{\mu_0} (b\phi(\nu) + c\nu^{-1/2}\phi(\nu)^{1/2})\,\mathrm{d}\nu.\end{aligned}$$

With $\Psi(\mu) \equiv \Phi(\mu)\mathrm{e}^{-b(\mu_0-\mu)}$, we easily compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\mu}\Psi(\mu) &= \left(b(\Phi(\mu) - \phi(\mu)) - c\mu^{-1/2}\phi(\mu)^{1/2}\right)\mathrm{e}^{-b(\mu_0-\mu)} \\ &\ge -c\mu^{-1/2}\phi(\mu)^{1/2}\mathrm{e}^{-b(\mu_0-\mu)} \\ &\ge -c\mu^{-1/2}\Phi(\mu)^{1/2}\mathrm{e}^{-b(\mu_0-\mu)}.\end{aligned}$$

Introducing $\psi(\mu) \equiv c\mu^{-1/2}\mathrm{e}^{-b(\mu_0-\mu)/2}$ we can rewrite this last inequality as

$$\frac{\mathrm{d}}{\mathrm{d}\mu}\Psi(\mu) \geq -\psi(\mu)\Psi(\mu)^{1/2},$$

and from this we get that

$$\frac{\mathrm{d}}{\mathrm{d}\mu}\Psi(\mu)^{1/2} \geq -\frac{1}{2}\psi(\mu).$$

After integration, we obtain

$$\Psi(\mu)^{1/2} \leq \Psi(\mu_0)^{1/2} + \frac{1}{2}\int_\mu^{\mu_0} \psi(\nu)\,\mathrm{d}\nu,$$

and since $\Psi(\mu_0) = \Phi(\mu_0) = \phi(\mu_0) + a\mu_0$,

$$\Psi(\mu)^{1/2} \leq (\phi(\mu_0) + a\mu_0)^{1/2} + \frac{c}{2}\int_\mu^{\mu_0} \nu^{-1/2}\mathrm{e}^{-b(\mu_0-\nu)/2}\,\mathrm{d}\nu.$$

Finally, we get

$$\begin{aligned}
\phi(\mu)^{1/2} &\leq \Phi(\mu)^{1/2} = \mathrm{e}^{b(\mu_0-\mu)/2}\Psi(\mu)^{1/2}\\
&\leq \mathrm{e}^{b\mu_0/2}(\phi(\mu_0) + a\mu_0)^{1/2} + \frac{c}{2}\int_0^{\mu_0} \nu^{-1/2}\mathrm{e}^{b(\nu-\mu)/2}\,\mathrm{d}\nu\\
&\leq \mathrm{e}^{b\mu_0/2}\left((\phi(\mu_0) + a\mu_0)^{1/2} + c\mu_0^{1/2}\right),
\end{aligned}$$

and it is straightforward to check that the same estimate is valid for $-\gamma < -\mu_0 < \mu < 0$. We have thus shown that $\sup_{\langle z,\mu\rangle\in\Omega_\gamma} \|TG_\mu(z)T\| < \infty$, and in particular that

$$\sup_{\mathrm{Re}\,(z)\in I, \mathrm{Im}\,(z)\neq 0} \|T(H-z)^{-1}T\| < \infty.$$

Invoking a covering argument, we easily show that, for any compact set $I \subset O \setminus \mathrm{Sp_{pp}}(H)$,

$$C(I) \equiv \sup_{\mathrm{Re}\,(z)\in I, \mathrm{Im}\,(z)\neq 0} \|T(H-z)^{-1}T\| < \infty. \tag{103}$$

Since $\mathrm{Ran}\,(T) = \mathrm{Dom}(A)$ is dense in $\mathscr{H}$, we can conclude that $I \cap \mathrm{Sp_{sc}}(H)$ is empty. □

4.3 Propagation estimates

The Mourre estimate provides a very efficient method to derive propagation estimates, which are essential ingredients of the time-dependent approach to scattering theory. We shall also use these estimates in our derivation of the Landauer-Büttiker formula.

The first result is a simple corollary of the proof of Theorem 4.25 (see [M2, M3]).

Corollary 4.26 *Let H be a self-adjoint operator on the Hilbert space $\mathscr{H}$. If H satisfies a Mourre estimate on the open set $O \subset \mathbb{R}$ with the conjugate operator A and if $H \in C^2_{\rm loc}(A)$ then, for any function $g \in C_0^\infty(O \setminus \mathrm{Sp}_{\rm pp}(H))$ there exists a constant C such that*

$$\int_{-\infty}^{\infty} \|(1+A^2)^{-1/2}\mathrm{e}^{-\mathrm{i}tH}g(H)u\|^2\,\mathrm{d}t \le C\,\|u\|^2, \tag{104}$$

for all $u \in \mathscr{H}$.

Proof. Let $g \in C_0^\infty(O \setminus \mathrm{Sp}_{\rm pp}(H))$ and set $I = \mathrm{supp}\, g$. The hypotheses of Theorem 4.25 being satisfied and $(1+|A|)^{-1}(1+A^2)^{1/2}$ being bounded, the inequality (103) implies

$$\sup_{\mathrm{Re}\,(z)\in I, \mathrm{Im}\,(z)\neq 0} \|(1+A^2)^{-1/2}(H-z)^{-1}(1+A^2)^{-1/2}\| < \infty.$$

It follows that $(1+A^2)^{-1/2}$ is H-smooth on I (compare with Eq. (12)). The operator $(A^2+1)^{-1/2}g(H)$ is thus H-smooth, and (104) follows. □

Our main tool in controlling the dynamics is the propagation estimate of Sigal-Soffer [SiSo] (see also [HSS] and Section 4.12 of [DG]). Recall that if A is a self-adjoint operator then $F(A \le a)$ denotes the spectral projection $E_{]-\infty,a]}(A)$, etc.

Proposition 4.27 *Let A and H be self-adjoint operators on the Hilbert space $\mathscr{H}$ such that:*

(i) $H \in C^n_{\rm loc}(A)$ *for an integer* $n \ge 2$.

(ii) *H satisfies a strict Mourre estimate with the conjugate operator A on the open set $O \subset \mathbb{R}$.*

Then, for all $s < n-1$ and $g \in C_0^\infty(O)$, there exist constants $\vartheta > 0$ and c such that

$$\|F(\pm A \le a - b + \vartheta t)\mathrm{e}^{\mp\mathrm{i}tH}g(H)F(\pm A \ge a)\| \le c\,\langle b + \vartheta t\rangle^{-s}, \tag{105}$$

for all $a \in \mathbb{R}$, $b \ge 0$ and $t \ge 0$.

5 Non-equilibrium steady states

In this section, we reconsider the problem of constructing nonequilibrium steady states for an open system of quasi-free fermions driven by extended reservoirs. Like the Authors of [AJPP2, N], we follow Ruelle's scattering approach [R2, R3]. The originality of the present work is in the use of time dependent scattering theory, inspired by the approach of Avron *et al.* to the related problem of adiabatic charge pumping [AEGSS].

The stationary approach to scattering used in [AJPP2, N] has the advantage of providing explicit representations of certain objects (Møller operators, scattering matrix). It thus allows for fairly simple and direct calculations. On the other hand, it requires quite strong assumptions,

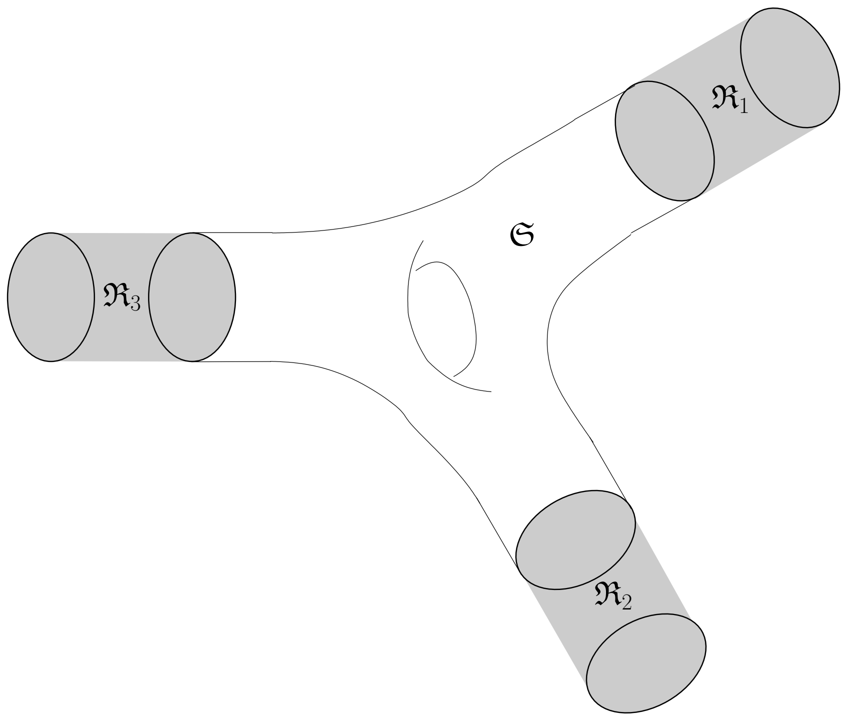

Figure 3: An ideal Fermi gas on a geometric structure $\mathfrak{M}$ structure.

specifically some trace conditions on the coupling between the system and the reservoir. Furthermore, it does not provide any control on the singular continuous spectrum. The absence of this spectral component is part of the assumptions of [AJPP2]. Our time-dependent approach is base on Mourre theory. It simultaneously gives us control over the singular spectrum, propagation estimates, and the property of local *Kato-Smoothness* which provide the construction of complete Møller operators and unitary scattering matrix.

5.1 Model and hypotheses

We consider an ideal Fermi gas confined to a connected geometric structure $\mathfrak{M}$. This structure may be a domain $\mathfrak{M} \subset \mathbb{R}^d$ or a finite dimensional Riemannian manifold which we shall assume is itself embedded in a Euclidean space $\mathbb{R}^d$. We shall suppose that $\mathfrak{M}$ is the disjoint union of a a compact subset $\mathfrak{S}$ and of M infinite tubular or cylindrical branches $\mathfrak{R}_1, \ldots \mathfrak{R}_M$ (see figure 3).

The fermions visiting the compact part $\mathfrak{S} \subset \mathfrak{M}$ form the small system $\mathscr{S}$. The reservoirs $\mathscr{R}_1, \ldots, \mathscr{R}_M$ consist in the fermions contained in the infinitely extended branches $\mathfrak{R}_1, \ldots, \mathfrak{R}_M$. In the context of mesoscopic physics, $\mathscr{S}$ is a sample connected to the electronic reservoirs $\mathscr{R}_k$. We denote by $\mathscr{H}$ the one-particle Hilbert space of the system, and by H its one-particle Hamiltonian, a self-adjoint operator on $\mathscr{H}$.

The system is described by the C^*-algebra $\mathscr{O} \equiv \mathrm{CAR}(\mathscr{H})$ equipped with the group of Bogoli-

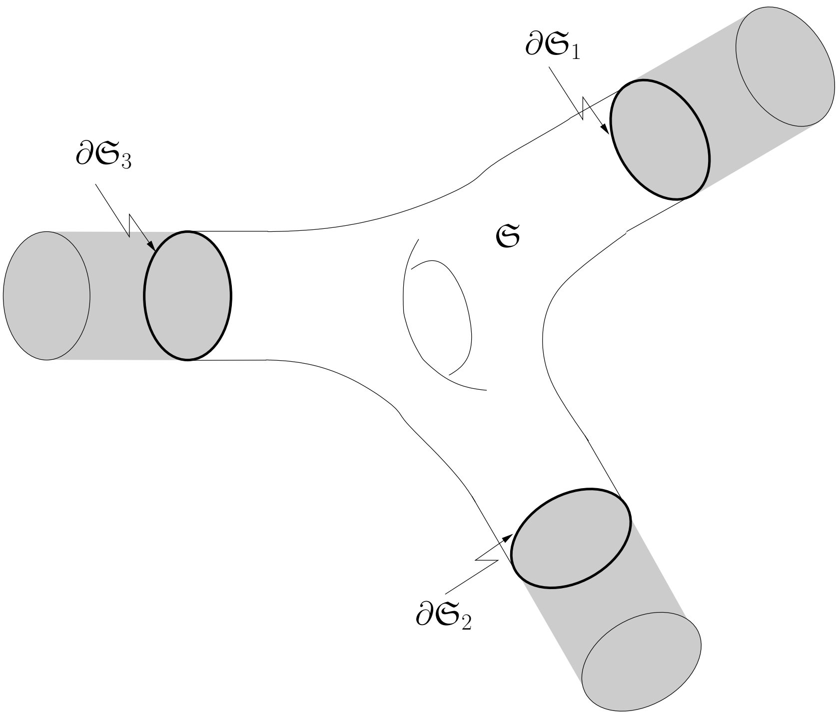

Figure 4: Decoupling of the sample $\mathfrak{S}$. Appropriate boundary conditions are imposed on the fictitious walls $\partial\mathfrak{S}_k$.

ubov automorphisms

$$\tau^t(a(f)) = a(\mathrm{e}^{\mathrm{i}tH} f).$$

To apply scattering theory to this system requires the definition of a reference dynamics. A possible approach consists in decoupling the compact part $\mathfrak{S}$ from the extended branches $\mathfrak{R}_k$ by imposing boundary conditions on fictitious walls $\partial\mathfrak{S}_k$ surrounding $\mathfrak{S}$ (see Figure 4). We then obtain a new Hamiltonian H_{ref} which will serve as reference. This is essentially the approach followed in [AJPP2] for example. However, this method has a serious disadvantage. In fact, the scattering matrix obtained in this way depends *a priori* on the largely arbitrary method used to perform the decoupling, i.e. the position of the decoupling walls, as well as the boundary conditions imposed at these walls. We shall avoid this difficulty by adopting a more geometric approach. We shall consider each reservoir as part of a larger system, a kind of super-reservoir, by immersing each branch $\mathfrak{R}_k$ in a reference structure $\widetilde{\mathfrak{R}}_k$ (see Figure 5). In this context, the two Hilbert spaces formalism of scattering theory applies. The advantage of this method is in the fact that the scattering matrix only depends on the geometry of the reservoirs and not on artificial decoupling techniques.

Let us now formulate our main hypotheses.

(H1) Submersion. For $k \in \{1, \ldots, M\}$ there exists a Hilbert space $\widetilde{\mathcal{H}}_k$ as well as a family of iden-

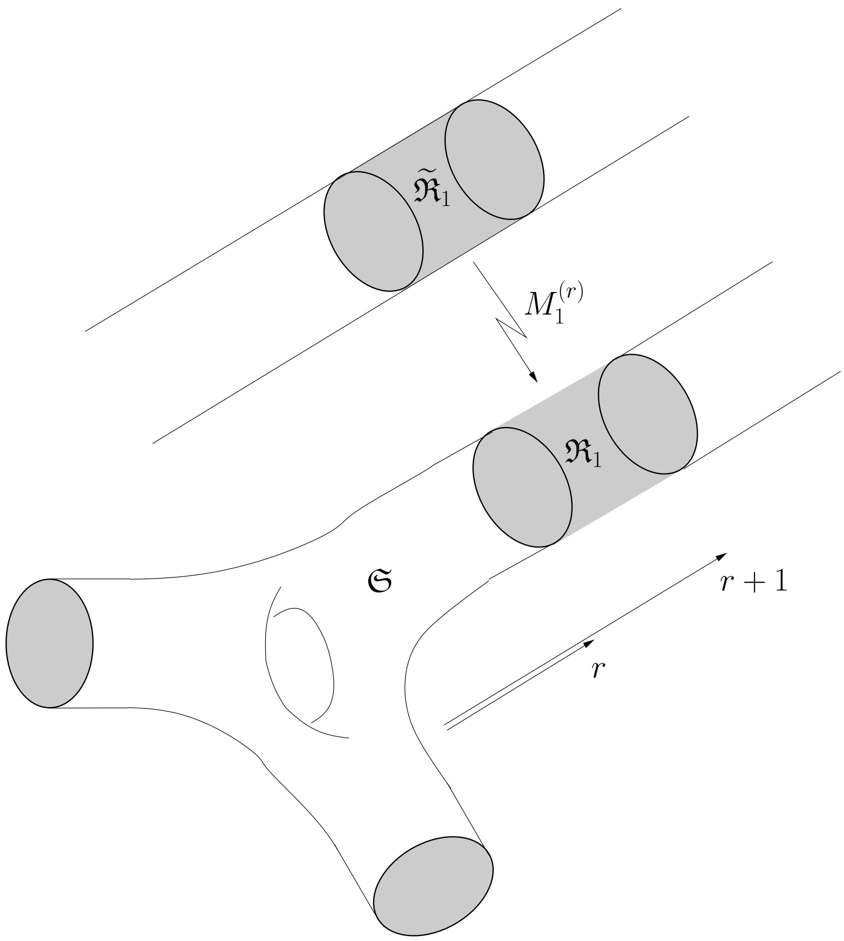

Figure 5: Submersion of the super-reservoir $\widetilde{\mathfrak{R}}_1$ into the extended branch $\mathfrak{R}_1$ of $\mathfrak{M}$. The parameter r describes the depth of this submersion.

tification operators $\{M_k^{(r)}\,|\,r\geq 0\}\subset\mathcal{B}(\widetilde{\mathcal{H}}_k,\mathcal{H})$. We denote by $M_k^{(r)}=J_k^{(r)}\widetilde{\chi}_k^{(r)}$ their polar decompositions, with $\widetilde{\chi}_k^{(r)}\equiv|M_k^{(r)}|=(M_k^{(r)*}M_k^{(r)})^{1/2}$. We also set $\chi_k^{(r)}\equiv(M_k^{(r)}M_k^{(r)*})^{1/2}$, $\tilde{1}_k^{(r)}\equiv J_k^{(r)*}J_k^{(r)}$ and $1_k^{(r)}\equiv J_k^{(r)}J_k^{(r)*}$. We assume that:

(i) $\|M_k^{(r)}\|=1$.

(ii) $\tilde{1}_k^{(r+1)}\leq\widetilde{\chi}_k^{(r)2}$ and $1_k^{(r+1)}\leq\chi_k^{(r)2}$.

(iii) $J_k^{(r)*}J_l^{(r)}=0$ for $k\neq l$.

(iv) $\tilde{1}_k^{(s)}\leq\tilde{1}_k^{(r)}$ if $0\leq r\leq s$ and $\mathrm{s}-\lim_{r\to\infty}\tilde{1}_k^{(r)}=0$.

(v) $1_k^{(s)}\leq 1_k^{(r)}$ if $0\leq r\leq s$ and $\mathrm{s}-\lim_{r\to\infty}1_k^{(r)}=0$.

(vi) $J_k^{(r)}\tilde{1}_k^{(s)}=1_k^{(s)}J_k^{(r)}=J_k^{(s)}$ for $0\leq r\leq s$.

$\widetilde{\mathcal{H}}_k$ is the Hilbert space of the super-reservoir and $M_k^{(r)}$ is the operator which maps one half of this super-reservoir $\widetilde{\mathcal{R}}_k$ into $\mathfrak{M}$. The parameter r describes the "depth" of this submersion. One can also think of r as describing the "position" of a fictitious interface between the system $\mathfrak{S}$ and the reservoir $\mathcal{R}_k$ (see Figure 5).

The properties of the polar decomposition imply that the operator $J_k^{(r)}$ is a partial isometry with initial space

$$\widetilde{\mathcal{H}}_k^{(r)}\equiv\mathrm{Ran}\,(M_k^{(r)*})^{\mathrm{cl}}=\mathrm{Ker}\,(M_k^{(r)})^{\perp}=\mathrm{Ran}\,(\widetilde{\chi}_k^{(r)})^{\mathrm{cl}}=\mathrm{Ker}\,(\widetilde{\chi}_k^{(r)})^{\perp}=\mathrm{Ran}\,(J_k^{(r)*})=\mathrm{Ker}\,(J_k^{(r)})^{\perp},$$

and final space

$$\mathcal{H}_k^{(r)}\equiv\mathrm{Ran}\,(M_k^{(r)})^{\mathrm{cl}}=\mathrm{Ker}\,(M_k^{(r)*})^{\perp}=\mathrm{Ran}\,(\chi_k^{(r)})^{\mathrm{cl}}=\mathrm{Ker}\,(\chi_k^{(r)})^{\perp}=\mathrm{Ran}\,(J_k^{(r)})=\mathrm{Ker}\,(J_k^{(r)*})^{\perp}.$$

$J_k^{(r)*}$ is the inverse isometry. $1_k^{(r)}$ is the orthogonal projection of $\mathcal{H}$ onto $\mathcal{H}_k^{(r)}$ while $\tilde{1}_k^{(r)}$ is the orthogonal projection of $\widetilde{\mathcal{H}}_k$ onto $\widetilde{\mathcal{H}}_k^{(r)}$. In particular, since $\widetilde{\chi}_k^{(r)}\geq 0$ and $\|\widetilde{\chi}_k^{(r)2}\|=\|M_k^{(r)*}M_k^{(r)}\|=\|M_k^{(r)}\|^2=1$ one has $0\leq\widetilde{\chi}_k^{(r)}\leq I$ and since $\mathrm{Ran}\,(\widetilde{\chi}_k^{(r)})^{\mathrm{cl}}=\mathrm{Ran}\,(\tilde{1}_k^{(r)})$ we easily verify the inequalities

$$0\leq\widetilde{\chi}_k^{(r)2}\leq\widetilde{\chi}_k^{(r)}\leq\tilde{1}_k^{(r)}\leq I,\qquad 0\leq\chi_k^{(r)2}\leq\chi_k^{(r)}\leq 1_k^{(r)}\leq I,\tag{106}$$

for $r\geq 0$. If $u\in\mathrm{Ran}\,\tilde{1}_k^{(r+1)}$ we deduce from (106) and Property (ii) that

$$0\leq(u,(I-\widetilde{\chi}_k^{(r)})u)\leq(u,(I-\widetilde{\chi}_k^{(r)2})u)=(u,(\tilde{1}_k^{(r+1)}-\widetilde{\chi}_k^{(r)2})u)\leq 0,$$

so that $(I-\widetilde{\chi}_k^{(r)2})u=0$. Since $(I-\widetilde{\chi}_k^{(r)})u=(I+\widetilde{\chi}_k^{(r)})^{-1}(I-\widetilde{\chi}_k^{(r)2})u=0$ we conclude that $\widetilde{\chi}_k^{(r)}\tilde{1}_k^{(r+1)}=\tilde{1}_k^{(r+1)}=\tilde{1}_k^{(r+1)}\widetilde{\chi}_k^{(r)}$ (the same identity is verified without the tildes). For $s\geq r+1\geq 1$ Properties (iv)-(v) yield $\tilde{1}_k^{(r+1)}\tilde{1}_k^{(s)}=\tilde{1}_k^{(s)}$ (and the same relation without the tildes), hence one has

$$\widetilde{\chi}_k^{(r)}\tilde{1}_k^{(s)}=\tilde{1}_k^{(s)}\widetilde{\chi}_k^{(r)}=\tilde{1}_k^{(s)},\qquad\chi_k^{(r)}1_k^{(s)}=1_k^{(s)}\chi_k^{(r)}=1_k^{(s)},\tag{107}$$

Property (iii) implies that $1_k^{(r)}1_l^{(r)} = \delta_{kl}1_k^{(r)}$. The operator $1_0^{(r)} = I - \sum_{j=1}^{M} 1_k^{(r)}$ is the orthogonal projection onto a neighborhood of "radius" r containing the system $\mathfrak{S}$.

We thus obtain a partition of unity on $\mathcal{H}$. We shall write

$$\mathcal{H} = \bigoplus_{k=0}^{M} \mathcal{H}_k^{(r)},$$

for the corresponding decomposition. By setting $\widetilde{\mathcal{H}}_0^{(r)} \equiv \mathcal{H}_0^{(r)}$ and $J_0^{(r)} = I$ we obtain a unitary

$$\begin{array}{rccc} U^{(r)}: & \widetilde{\mathcal{H}} \equiv \oplus_{k=0}^{M} \widetilde{\mathcal{H}}_k^{(r)} & \to & \mathcal{H} \\ & (u_0, \dots, u_M) & \mapsto & \sum_{j=0}^{M} J_k^{(r)} u_k, \end{array}$$

with inverse

$$\begin{array}{rccc} U^{(r)*}: & \mathcal{H} & \to & \widetilde{\mathcal{H}} \\ & u & \mapsto & (J_0^{(r)*} u, \dots, J_M^{(r)*} u). \end{array}$$

(H2) Coupling. For $k \in \{1, \dots, M\}$ there exists a self-adjoint Hamiltonian $\widetilde{H}_k$ on $\widetilde{\mathcal{H}}_k$ such that

(i) $M_k^{(r)}\mathrm{Dom}(\widetilde{H}_k) \subset \mathrm{Dom}(H)$ and $M_k^{(r)*}\mathrm{Dom}(H) \subset \mathrm{Dom}(\widetilde{H}_k)$.

(ii) H "coincides" with $\widetilde{H}_k$ on $M_k^{(r)}\mathrm{Dom}(\widetilde{H}_k)$:

$$HM_k^{(r)}u = J_k^{(r)}\widetilde{H}_k\widetilde{\chi}_k^{(r)}u,$$

for all $u \in \mathrm{Dom}(\widetilde{H}_k)$.

(iii) $(I - \tilde{1}_k^{(r)})\widetilde{H}_k\widetilde{\chi}_k^{(r)}u = 0$ for all $u \in \mathrm{Dom}(\widetilde{H}_k)$ and $r \geq 0$.

(iv) The operator $B_k^{(r)} \equiv [\widetilde{H}_k, \widetilde{\chi}_k^{(r)}]$ is $\widetilde{H}_k$-compact.

(v) The operator $B_k^{(r)*}J_k^{(r)*}$ is H-compact.

(vi) For all $r \geq 0$, $1_0^{(r)}$ is H-compact.

(vii) For all $r, s \geq 0$, $\tilde{1}_k^{(r)} - \tilde{1}_k^{(s)}$ is $\widetilde{H}_k$-compact.

We note that condition (iii) and Hypothesis (H1) (ii) imply that if $s \geq r + 1 \geq 1$ then

$$\widetilde{\chi}_k^{(s)}\widetilde{H}_k(I - \widetilde{\chi}_k^{(r)})u = (I - \widetilde{\chi}_k^{(r)})\widetilde{H}_k\widetilde{\chi}_k^{(s)}u = 0, \tag{108}$$

for all $u \in \mathrm{Dom}(\widetilde{H}_k)$.

Finally our main hypothesis ensures good propagation properties in the reservoirs. We shall denote by $\widetilde{\mathcal{H}}_k^1$ the space $\mathrm{Dom}(\widetilde{H}_k)$ equipped with the graph norm and $\widetilde{\mathcal{H}}_k^{-1}$ its dual (see Definition 4.13).

(H3) Mourre estimate. For $k \in \{1,\dots,M\}$ there exists a self-adjoint operator $\widetilde{A}_k$ on $\widetilde{\mathscr{H}}_k$ and a closed, countable subset $\Sigma_k \subset \mathbb{R}$ such that for any $E \in \mathbb{R}\setminus\Sigma_k$, $\widetilde{H}_k$ satisfies a Mourre estimate at E with the conjugate operator $\widetilde{A}_k$. Furthermore:

(i) $\widetilde{\chi}_k^{(r)}\mathrm{Dom}(\widetilde{A}_k) \subset \mathrm{Dom}(\widetilde{A}_k)$ for all $r \geq 0$.

(ii) $[\widetilde{A}_k, \widetilde{\chi}_k^{(r)}] = 0$ for $r \in [0,2]$.

(iii) $(\tilde{1}_k^{(0)} - \widetilde{\chi}_k^{(r)})\widetilde{A}_k = 0$ for $r \in [0,2]$.

(iv) $\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}\mathrm{Dom}(\widetilde{H}_k) \subset \mathrm{Dom}(\widetilde{H}_k)$ for $\theta \in \mathbb{R}$.

(v) $\widetilde{H}_k \in \mathscr{B}^n_{\widetilde{A}_k}(\widetilde{\mathscr{H}}_k^1, \widetilde{\mathscr{H}}_k)$ for some integer $n \geq 2$.

5.2 A simple model

In this section we illustrate our Hypotheses (H1)–(H3) with a simple non-trivial example. We also discuss various possible extensions and modifications of this example.

Let $\mathfrak{M}$ be a smooth 2-dimensional connected sub-manifold of $\mathbb{R}^3$ such that $\mathfrak{M} = \mathfrak{S} \cup \mathfrak{R}_- \cup \mathfrak{R}_+$ where $\mathfrak{S}$ is compact with boundary $\partial\mathfrak{S} = \gamma_- \cup \gamma_+$ where

$$\gamma_\mp = \left\{x = (x_1, x_2, \mp 1) \in \mathbb{R}^3 \,\middle|\, x_1^2 + x_2^2 = R^2\right\},$$

and $\mathfrak{R}_\mp$ are semi-infinite cylinders

$$\mathfrak{R}_\mp = \left\{x = (x_1, x_2, x_3) \in \mathbb{R}^3 \,\middle|\, x_1^2 + x_2^2 = R^2, \mp x_3 > 1\right\},$$

The super-reservoirs are infinite cylinders

$$\widetilde{\mathfrak{R}}_\mp = \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_1^2 + x_2^2 = R^2\},$$

and for $r \geq 0$ we set $\mathfrak{R}_\mp^{(r)} = \{x \in \mathfrak{R}_\mp \mid \mp x_3 \geq 1 + r\} \subset \mathfrak{M} \cap \widetilde{\mathfrak{R}}_\mp$.

The various Hilbert spaces are just the corresponding L^2-spaces with the induced surface measures, e.g., $\mathscr{H} = L^2(\mathfrak{M})$. The operator $M_+^{(r)}$ is defined by

$$(M_+^{(r)} f)(x_1, x_2, x_3) = \begin{cases} g(x_3 - 1 - r) f(x_1, x_2, x_3) & \text{if } (x_1, x_2, x_3) \in \mathfrak{R}_+, \\ 0 & \text{otherwise,} \end{cases}$$

where $g \in C^\infty(\mathbb{R})$ is such that $0 \leq g(x) \leq 1$, $g(x) = 0$ for $x \leq 0$ and $g(x) = 1$ for $x \geq 1$. A similar definition holds for $M_-^{(r)}$. One easily checks that $\widetilde{\chi}_+^{(r)}$ is the operator of multiplication by the function $g(x_3 - 1 - r)$ on the Hilbert space $L^2(\widetilde{\mathfrak{R}}_+)$ while $\chi_1^{(r)}$ is the operator of multiplication by the function $1_{\mathfrak{R}_+}(x) g(x_3 - 1 - r)$ on the Hilbert spaces $L^2(\mathfrak{M})$ where $1_{\mathfrak{R}_+}$ denotes the indicator function of $\mathfrak{R}_+ \subset \mathfrak{M}$. The partial isometry $J_\mp^{(r)} : L^2(\widetilde{\mathfrak{R}}_\mp) \to L^2(\mathfrak{M})$ is given by

$$(J_\mp^{(r)} u)(x) = \begin{cases} u(x) & \text{if } x \in \mathfrak{R}_\mp^{(r)}, \\ 0 & \text{if } x \in \mathfrak{M} \setminus \mathfrak{R}_\mp^{(r)}, \end{cases}$$

and its adjoint $J_{\mp}^{(r)*}: L^2(\mathfrak{M}) \to L^2(\widetilde{\mathfrak{R}}_{\mp})$ acts as

$$(J_{\mp}^{(r)*} u)(x) = \begin{cases} u(x) & \text{if } x \in \mathfrak{R}_{\mp}^{(r)}, \\ 0 & \text{if } x \in \widetilde{\mathfrak{R}}_1 \setminus \mathfrak{R}_{\mp}^{(r)}. \end{cases}$$

The orthogonal projection $1_{\mp}^{(r)}$ (resp. $\widetilde{1}_{\mp}^{(r)}$) acts on $L^2(\mathfrak{M})$ (resp. on $L^2(\widetilde{\mathfrak{R}}_{\mp})$) as multiplication with the indicator function of the subset $\mathfrak{R}_{\mp}^{(r)}$. It is a simple exercise to verify Properties (i)–(vi) of Hypothesis (H1).

Denote by $\Delta_{\mathfrak{M}}$ the Laplace-Beltrami operator acting on $\mathscr{D}_{\mathfrak{M}} = C_0^\infty(\mathfrak{M})$. If $q = (q_1, q_2)$ are local coordinates on some open subset $\mathfrak{Q} \subset \mathfrak{M}$ then $\Delta_{\mathfrak{M}}$ acts on $C_0^\infty(\mathfrak{Q})$ as the second order, elliptic differential operator

$$\sum_{i,j=1}^{2} g(q)^{-1/2} \partial_{q_i} g(q)^{1/2} g^{ij}(q) \partial_{q_j},$$

where g denotes the determinant of the metric tensor $[g_{ij}]$ and $[g^{ij}]$ its inverse. In particular $\Delta_{\mathfrak{M}}$ maps $\mathscr{D}_{\mathfrak{M}}$ into itself. Since the surface measure is given locally on $\mathfrak{Q}$ by $\mathrm{d}\sigma = g(q)^{1/2} \mathrm{d}q_1 \mathrm{d}q_2$, one easily checks that $\Delta_{\mathfrak{M}}$ is symmetric as an operator on $L^2(\mathfrak{M})$ with domain $\mathscr{D}_{\mathfrak{M}}$. We denote by the same symbol the dual action of $\Delta_{\mathfrak{M}}$ on the space $\mathscr{D}'(\mathfrak{M})$ of distributions on $\mathfrak{M}$ (the duality being induced by the inner product of $L^2(\mathfrak{M})$).

In fact, the operator $-\Delta_{\mathfrak{M}}$ is essentially self-adjoint on $\mathscr{D}_{\mathfrak{M}}$ (see, e.g., [Ch, Co, D5, Str]) and we denote by H its self-adjoint extension. Explicitly, the domain of H is given by $\mathrm{Dom}(H) = \{u \in \mathscr{H} \,|\, \Delta_{\mathfrak{M}} u \in \mathscr{H}\}$ and for $u \in \mathrm{Dom}(H)$ one has $Hu = -\Delta_{\mathfrak{M}} u$ in distributional sense. Moreover, H is positive and its quadratic form is the Dirichlet form

$$(u, Hu) = \int_{\mathfrak{M}} |\nabla u|^2 \mathrm{d}\sigma,$$

where ∇ denotes the gradient operator (in local coordinates $\nabla^i = \sum_j g^{ij}(q) \partial_{q_j}$). The same conclusions hold for the Laplace-Beltrami operator $\Delta_{\widetilde{\mathfrak{R}}_{\mp}}$ acting on $C_0^\infty(\widetilde{\mathfrak{R}}_{\mp})$ and we denote by $\widetilde{H}_{\mp}$ the self-adjoint extension of $-\Delta_{\widetilde{\mathfrak{R}}_{\mp}}$. It is now straightforward to verify Properties (i)–(iii) of Hypothesis (H2). Properties (iv)–(vii) easily follow from the fact that the weighted Sobolev space

$$H_w^s(\mathfrak{M}) = \{u \in \mathrm{Dom}(H^{s/2}) \,|\, w H^{s/2} u \in L^2(\mathfrak{M})\},$$

with $s > 0$ is compactly embedded in $L^2(\mathfrak{M})$ if the weight $w \in C^\infty(\mathfrak{M})$ is such that

$$\lim_{|x_3| \to \infty} w(x) = +\infty,$$

(and a similar statement for $H_w^s(\widetilde{\mathfrak{R}}_{\mp})$), see, e.g. [Lo]).

We note that $\widetilde{\mathscr{H}}_{\mp} = L^2(\mathbb{R} \times \gamma_{\mp}, \mathrm{d}x\, R\mathrm{d}\varphi)$, where $R\mathrm{d}\varphi$ is the arc-length measure on the circle $\gamma_{\mp}$, and that

$$\widetilde{H}_{\mp} = -\partial_x^2 + \Lambda^2, \qquad \Lambda^2 = -R^{-2} \partial_\varphi^2.$$

Set $\Sigma_\mp = \mathrm{Sp}(\Lambda^2) = \{\lambda_n^2 = n^2/R^2 \,|\, n \in \mathbb{N}\}$ and let $v \in C^\infty(\mathbb{R})$ be such that $v(x) = 0$ for $|x| \le 5$, $v'(x) \ge 0$ and $v(x) = x$ for $|x| \ge 15$. Denote by Φ^t the global flow defined by the ODE $\dot{x} = v(x)$ and set $j^t = (\partial_x \Phi^t)^{1/2}$. The operators defined by $(U^t u)(x,\varphi) = j^t(x)u(\Phi^t(x),\varphi)$ form a strongly continuous unitary group on $\widetilde{\mathscr{H}}_\mp$ leaving the subspaces $C_0^\infty(\widetilde{\mathfrak{R}}_\mp)$ as well as $\mathrm{Dom}(\widetilde{H}_\mp)$ invariants. Define $\widetilde{A}_\mp$ to be its self-adjoint generator. One easily checks that $C_0^\infty(\widetilde{\mathfrak{R}}_\mp)$ is in the domain of $\widetilde{A}_\mp$ and that

$$\widetilde{A}_\mp = \frac{1}{2\mathrm{i}}\left(v(x)\partial_x + \partial_x v(x)\right),$$

on this subspace. By the core theorem, $\widetilde{A}_\mp$ is essentially self-adjoint on $C_0^\infty(\widetilde{\mathfrak{R}}_\mp)$ and hence acts in the same way, in the sense of distributions, on its domain $\mathrm{Dom}(\widetilde{A}_\mp) = \{u \in \widetilde{\mathscr{H}}_\mp \,|\, \widetilde{A}_\mp u \in \widetilde{\mathscr{H}}_\mp\}$.

A formal calculation shows that

$$\mathrm{i}[\widetilde{H}_\mp, \widetilde{A}_\mp] = 2(\widetilde{H}_\mp - \Lambda^2) + 2\partial_x(1 - v'(x))\partial_x - \frac{1}{2}v'''(x),$$

which defines a bounded quadratic form on $\mathrm{Dom}(\widetilde{H}_\mp)$. Applying Theorem 4.22 we conclude that $\widetilde{H}_\mp$ is of class $C^1_{\mathrm{loc}}(\widetilde{A}_\mp)$ and Lemma 4.16 yields that

$$1_\Delta(\widetilde{H}_\mp)\mathrm{i}[\widetilde{H}_\mp, \widetilde{A}_\mp]1_\Delta(\widetilde{H}_\mp) = 1_\Delta(\widetilde{H}_\mp)\left(2(\widetilde{H}_\mp - \Lambda^2) + 2\partial_x(1 - v'(x))\partial_x - \frac{1}{2}v'''(x)\right)1_\Delta(\widetilde{H}_\mp),$$

is self-adjoint for any bounded interval $\Delta \subset \mathbb{R}$. Let $E \in \mathbb{R} \setminus \Sigma_\mp$ so that $\theta = \mathrm{dist}(E, \Sigma_\mp) > 0$ (see Figure 6). With $\Delta = [E - \theta/2, E + \theta/2]$, it follows from the functional calculus that

$$1_\Delta(\widetilde{H}_\mp)2(\widetilde{H}_\mp - \Lambda^2)1_\Delta(\widetilde{H}_\mp) \ge \theta 1_\Delta(\widetilde{H}_\mp).$$

Moreover, since $1 - v'$ and v''' belong to $C_0^\infty(\mathbb{R})$, Rellich's criterion yields that

$$K_\mp = 1_\Delta(\widetilde{H}_\mp)\left(2\partial_x(1 - v'(x))\partial_x - \frac{1}{2}v'''(x)\right)1_\Delta(\widetilde{H}_\mp),$$

is compact. Thus, one has

$$1_\Delta(\widetilde{H}_\mp)\mathrm{i}[\widetilde{H}_\mp, \widetilde{A}_\mp]1_\Delta(\widetilde{H}_\mp) \ge \theta 1_\Delta(\widetilde{H}_\mp) + K_\mp,$$

which shows that $\widetilde{H}_\mp$ satisfies a Mourre estimate with conjugate operator $\widetilde{A}_\mp$ at every $E \in \mathbb{R} \setminus \Sigma_\mp$. Properties (i)–(iv) of Hypothesis (H3) are now easily verified. A simple induction argument shows that for any integer $n \ge 1$ one has

$$\mathrm{ad}^{\mathrm{n}}_{\tilde{\mathrm{A}}_\mathrm{j}}(\tilde{\mathrm{H}}_\mathrm{j}) = -\partial_\mathrm{x}(2^\mathrm{n} + \mathrm{a}_\mathrm{n}(\mathrm{x}))\partial_\mathrm{x} + \mathrm{b}_\mathrm{n}(\mathrm{x}),$$

with $a_n, b_n \in C_0^\infty(\widetilde{\mathfrak{R}}_\mp)$. Lemma 4.21 allows us to conclude that Hypothesis (H3) (v) holds for any integer $n \ge 0$.

This simple example can be modified in a number of ways by straightforward adaptations of the above discussion:

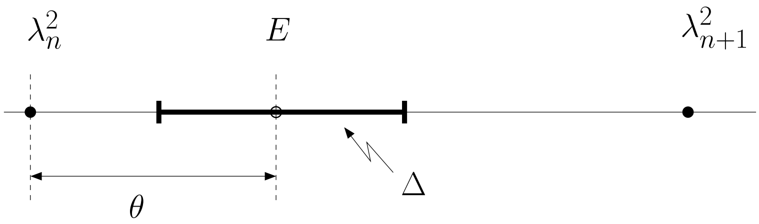

Figure 6: If $E \notin \Sigma_\mp = \{\lambda_k^2\}_{k\in\mathbb{N}}$, one can chose Δ such that $\mathrm{dist}(\Sigma_\mp, \Delta) = \theta/2 > 0$.

- The manifold $\mathfrak{M}$ can have more that two cylindrical ends $\mathfrak{R}_j$.
- The cylindrical ends $\mathfrak{R}_j$ can have arbitrary, smooth, compact bases γ_j with metric g_{γ_j}.
- The dimension of $\mathfrak{M}$ can be arbitrary, as long as this smooth manifold is the union of a compact piece $\mathfrak{S}$ and a finite number of cylindrical ends of the type $\mathfrak{R}_j =]1, \infty[\times \gamma_j$ with the metric $g_{\mathfrak{R}_j} = \mathrm{d}x^2 + g_{\gamma_j}$.
- A potential $V : \mathfrak{S} \to \mathbb{R}$ can be added to the Hamiltonian H.
- The metric on the cylindrical ends of the manifold $\mathfrak{M}$ can be slightly perturbed.

Scattering theory on non-compact complete Riemannian manifolds with Euclidean or hyperbolic metric near infinity has been intensively studied. Most of the cases covered by these studies can be casted within our framework. We refer the reader to [Hi, IKL, RT] for the development of scattering theory on manifolds with cylindrical ends.

A more radical change of the metric of the reservoirs leads to the concept of scattering manifold with super-reservoirs of the type $\widetilde{\mathfrak{R}}_j =]1, \infty[\times \gamma_j$ equipped with a metric $g_{\widetilde{\mathfrak{R}}_j} = \mathrm{d}x^2 + r(x)^2 g_{\gamma_j}$, such that $r(x) \to \infty$ as $x \to \infty$. The method used in these notes to derive the Landauer-Büttiker formula does not apply to this class of models, for this reason we will not consider them here and refer the interested reader to [Hi, IN, IS, Ku, MS] for discussions of the scattering theory. We note however that extending our results to this context is an interesting open problem.

5.3 The Mourre estimate

In this section we construct a conjugate operator for H, in the sense of Mourre estimate. To simplify our notation, we shall set $M_k \equiv M_k^{(1)}$, $J_k \equiv J_k^{(1)}$, $\widetilde{\chi}_k \equiv \widetilde{\chi}_k^{(1)}$, $\chi_k \equiv \chi_k^{(1)}$, $1_k \equiv 1_k^{(1)}$, $\tilde{1}_k \equiv \tilde{1}_k^{(1)}$, $\mathscr{H}_k \equiv \mathscr{H}_k^{(1)}$, and $U \equiv U^{(1)}$ for all $k \in \{0, \dots, M\}$.

Lemma 5.1 *If Hypotheses (H1) and (H3) are satisfied, the operator A defined by*

$$A \equiv \sum_{k=1}^{M} J_k \widetilde{A}_k J_k^*,$$

on $\mathrm{Dom}(A) \equiv \{u \in \mathscr{H} \,|\, J_k^* u \in \mathrm{Dom}(\widetilde{A}_k), k = 1, \ldots, M\}$ *is self-adjoint. Furthermore,* A *is reduced by the orthogonal projection* 1_k*,*

$$[\mathrm{e}^{\mathrm{i}\theta A}, 1_k] = 0, \quad k \in \{0, \ldots, M\}, \theta \in \mathbb{R}.$$

For $k \in \{0, \ldots, M\}$ *we set* $A_k \equiv A 1_k$*. These self-adjoint operators satisfy* $A_k = 1_k A 1_k = J_k \widetilde{A}_k J_k^* = M_k \widetilde{A}_k M_k^*$ *and* $A_0 = 0$*.*

Remark 5.1 The sample $\mathfrak{S}$, being localized in $\mathrm{Ran}\, 1_0$, it is also localized in $\mathrm{Ran}\, F(A = 0)$. For $a > 0$, $\mathrm{Ran}\, F(\pm A_k > a) \subset \mathrm{Ran}\, 1_k$, which leads to $F(\pm A_k > a)$ being localized in the interior of the reservoir $\mathscr{R}_k$. This fact will be very useful for the calculations of currents in the reservoirs.

Theorem 5.2 *Under Hypotheses (H1), (H2) and (H3), we have*

(i) $\mathrm{e}^{\mathrm{i}\theta A_k}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$ *and* $\mathrm{e}^{\mathrm{i}\theta A}\mathrm{Dom}(H) \subset \mathrm{Dom}(H)$ *for all* $\theta \in \mathbb{R}$ *and* $k \in \{1, \ldots, M\}$*.*

(ii) $H \in \mathscr{B}^n_{A_k}(\mathscr{H}^1_H, \mathscr{H})$ *for* $k \in \{1, \ldots, M\}$*.*

(iii) $H \in C^n_{\mathrm{loc}}(A)$*.*

(iv) There exists a closed and countable set $\Sigma_H \subset \mathbb{R}$ *such that* H *satisfies a strict Mourre estimate on* $\mathbb{R} \setminus \Sigma_H$ *with the conjugate operator* A*.*

Corollary 5.3 *Under the hypotheses of Theorem 5.2 we have*

(i) $\mathrm{Sp}_{\mathrm{sc}}(\widetilde{H}_k)$ *is empty for* $k \in \{1, \ldots, M\}$*.*

(ii) $\mathrm{Sp}_{\mathrm{pp}}(\widetilde{H}_k) \subset \Sigma_k$*.*

(iii) $\mathrm{Sp}_{\mathrm{sc}}(H)$ *is empty.*

(iv) $\mathrm{Sp}_{\mathrm{pp}}(H) \subset \Sigma_H$

The remaining of this section is devoted to the proofs of these important results.

Proof of Lemma 5.1. We begin by showing that for $k \in \{1, \ldots, M\}$ the orthogonal projection $\tilde{1}_k$ reduces $\widetilde{A}_k$. In fact Hypotheses (H3) (i) and (ii) imply that for all $u \in \mathrm{Dom}(\widetilde{A}_k)$ and $r \in [0, 2]$,

$$\frac{\mathrm{d}}{\mathrm{d}\theta} \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} \widetilde{\chi}_k^{(r)} \mathrm{e}^{-\mathrm{i}\theta \widetilde{A}_k} u = 0,$$

and consequently $[\widetilde{\chi}_k^{(r)}, \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k}] = 0$. Hypotheses (H1) (iv) and (H3) (iii) allow us to write

$$\frac{\mathrm{d}}{\mathrm{d}\theta} (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(s)}) \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} u = 0,$$

for all $u \in \mathrm{Dom}(\widetilde{A}_k)$ and $0 \le r \le s \le 2$. From this we get that $(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(s)}) \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(s)})$. By taking the adjoint we get

$$\mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(s)}) = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(s)}) = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(s)}) \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k}, \tag{109}$$

and in particular $[\tilde{1}_k^{(r)} - \tilde{\chi}_k^{(r)}, \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k}] = 0$. By combining this identity with the previous result we conclude that $[\tilde{1}_k^{(r)}, \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k}] = 0$, that is to say that $\tilde{1}_k^{(r)}$ reduces $\widetilde{A}_k$.
We denote by $\widetilde{A}_k^+$ the restriction of the operator $\widetilde{A}_k$ to the subspace $\mathrm{Ran}(\tilde{1}_k)$. This operator is self-adjoint on $\mathrm{Dom}(\widetilde{A}_k^+) = \tilde{1}_k \mathrm{Dom}(\widetilde{A}_k)$. We also set $\tilde{A}_0^+ \equiv 0$. We finish the proof by remarking that

$$A = U\left(\bigoplus_{k=0}^{M} \tilde{A}_k^+\right)U^*, \qquad 1_k = U\tilde{1}_k U^*.$$

□

To prove Theorem 5.2 we will need several lemmas. We shall denote by $R(z) \equiv (H-z)^{-1}$ and $\widetilde{R}_k(z) \equiv (\widetilde{H}_k - z)^{-1}$ the resolvents of H and of $\widetilde{H}_k$.

Lemma 5.4 (Resolvent equation) *If Hypotheses (H1) and (H2) are satisfied, then, for all $r \geq 0$ and all $z \in \mathrm{Res}(H) \cap \mathrm{Res}(\widetilde{H}_k)$, we have*

$$M_k^{(r)} \widetilde{R}_k(z) - R(z) M_k^{(r)} = R(z) J_k^{(r)} B_k^{(r)} \widetilde{R}_k(z).$$

Proof. Hypotheses (H2) (i)-(ii) yield $J_k^{(r)} B_k^{(r)} u = (H-z) M_k^{(r)} u - M_k^{(r)} (\widetilde{H}_k - z) u$ for all $u \in \mathrm{Dom}(\widetilde{H}_k)$. Thus, for all $u, v \in \mathscr{H}$ one has

$$\begin{aligned}(u, R(z) J_k^{(r)} B_k^{(r)} \widetilde{R}_k(z) v) &= (R(\overline{z}) u, (H-z) M_k^{(r)} \widetilde{R}_k(z) v) - (R(\overline{z}) u, M_k^{(r)} (\widetilde{H}_k - z) \widetilde{R}_k(z) v) \\ &= (u, M_k^{(r)} \widetilde{R}_k(z) v) - (R(\overline{z}) u, M_k^{(r)} v) = (u, M_k^{(r)} \widetilde{R}_k(z) v) - (u, R(z) M_k^{(r)} v).\end{aligned}$$

□

Corollary 5.5 *Suppose that Hypotheses (H1) and (H2) are satisfied. For all $f \in C_0^\infty(\mathbb{R})$, define the operator $D_k^{(r)}(f) \equiv f(H) M_k^{(r)} - M_k^{(r)} f(\widetilde{H}_k)$.*

(i) $D_k^{(r)}(f)$ is compact.

(ii) If Hypothesis (H3) is also satisfied then $D_k^{(r)}(f)[\widetilde{A}_k, \widetilde{H}_k]$ is compact.

Proof. (i) With the help of Lemma 5.4 we obtain, by using the Helffer-Sjöstrand formula,

$$D_k^{(r)}(f) = -\frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \overline{\partial} \tilde{f}(z) \, R(z) J_k^{(r)} B_k^{(r)} \widetilde{R}_k(z) \, \mathrm{d}z \wedge \mathrm{d}\overline{z}, \tag{110}$$

for an appropriate almost-analytic extension $\tilde{f}$ of f. Lemma 5.4 yields the bound

$$\| R(z) J_k^{(r)} B_k^{(r)} \widetilde{R}_k(z) \| \leq 2 \, |\mathrm{Im} z|^{-1},$$

which shows that the integral (110) converges in norm. The first resolvent equation further gives

$$R(z) J_k^{(r)} B_k^{(r)} \widetilde{R}_k(z) = R(z) J_k^{(r)} B_k^{(r)} \widetilde{R}_k(\mathrm{i})(I + (z - \mathrm{i}) \widetilde{R}_k(z)),$$

and $B_k^{(r)}\widetilde{R}_k(\mathrm{i})$ being compact by Hypothesis (H2) (iv), we conclude that $R(z)J_k^{(r)}B_k^{(r)}\widetilde{R}_k(z)$ is compact for $z\in\mathbb{C}\setminus\mathbb{R}$. Consequently, $D_k^{(r)}(f)$ is compact.

(ii) First, $[\widetilde{A}_k,\widetilde{H}_k]\in\mathscr{B}(\widetilde{\mathscr{H}}_k^1,\widetilde{\mathscr{H}}_k)$ by Hypothesis (H3) (v), implies $[\widetilde{H}_k,\widetilde{A}_k]=[\widetilde{A}_k,\widetilde{H}_k]^*\in\mathscr{B}(\widetilde{\mathscr{H}}_k,\widetilde{\mathscr{H}}_k^{-1})$ and thus

$$\widetilde{R}_k(z)[\widetilde{H}_k,\widetilde{A}_k]=(I+(z-\mathrm{i})\widetilde{R}_k(z))\widetilde{R}_k(\mathrm{i})[\widetilde{H}_k,\widetilde{A}_k],$$

is bounded on $\widetilde{\mathscr{H}}_k$. Furthermore, there exists a constant c such that

$$\|\widetilde{R}_k(z)[\widetilde{H}_k,\widetilde{A}_k]\|\le c\,|\mathrm{Im}z|^{-1},$$

for $z\in\operatorname{supp}\tilde{f}$.

Second,

$$R(z)J_k^{(r)}B_k^{(r)}=(I+(z+\mathrm{i})R(z))R(-\mathrm{i})J_k^{(r)}B_k^{(r)}=(I+(z+\mathrm{i})R(z))(B_k^{(r)*}J_k^{(r)*}R(\mathrm{i}))^*,$$

is compact by Hypothesis (H2) (v) and there exists a constant c' such that

$$\|R(z)J_k^{(r)}B_k^{(r)}\|\le c'\,|\mathrm{Im}z|^{-1},$$

for $z\in\operatorname{supp}\tilde{f}$. We may conclude that the integral

$$D_k^{(r)}(f)[\widetilde{A}_k,\widetilde{H}_k]=-\frac{1}{2\pi}\int_{\mathbb{C}}\bar{\partial}\tilde{f}\,R(z)J_k^{(r)}B_k^{(r)}\widetilde{R}_k(z)[\widetilde{A}_k,\widetilde{H}_k]\,\mathrm{d}z\wedge\mathrm{d}\bar{z},$$

converges in norm and is compact. □

Lemma 5.6 *Under Hypotheses (H1) and (H3), for* $r\in[0,2]$ *and* $k\in\{1,\dots,M\}$ *we have*

$$J_k^{(r)}\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}J_k^{(r)*}=M_k^{(r)}\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}M_k^{(r)*}+1_k^{(r)}-M_k^{(r)}M_k^{(r)*},\tag{111}$$

for $\theta\in\mathbb{R}$. *Furthermore, for all* $j,l\in\mathbb{N}$, *and* $u\in\mathrm{Dom}(\widetilde{A}_k^l)$,

$$\tilde{1}_k^{(r)}\widetilde{A}_k^l u=\widetilde{\chi}_k^{(r)j}\widetilde{A}_k^l u=\widetilde{A}_k^l\widetilde{\chi}_k^{(r)j}u.\tag{112}$$

Proof. Since $J_k^{(r)}\tilde{1}_k^{(r)}=J_k^{(r)}$ and $J_k^{(r)}\tilde{1}_k^{(r)}J_k^{(r)*}=1_k^{(r)}$, the identity (109) allows us to write

$$\begin{aligned}J_k^{(r)}\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}J_k^{(r)*}&=J_k^{(r)}\widetilde{\chi}_k^{(r)}\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}J_k^{(r)*}+J_k^{(r)}(\tilde{1}_k^{(r)}-\chi_k^{(r)})J_k^{(r)*}\\&=J_k^{(r)}\widetilde{\chi}_k^{(r)}\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}\chi_k^{(r)}J_k^{(r)*}+J_k^{(r)}\widetilde{\chi}_k^{(r)}(\tilde{1}_k^{(r)}-\chi_k^{(r)})J_k^{(r)*}+J_k^{(r)}(\tilde{1}_k^{(r)}-\chi_k^{(r)})J_k^{(r)*}\\&=M_k^{(r)}\mathrm{e}^{\mathrm{i}\theta\widetilde{A}_k}M_k^{(r)*}+J_k^{(r)}\widetilde{\chi}_k^{(r)}J_k^{(r)*}-M_k^{(r)}M_k^{(r)*}+\tilde{1}_k^{(r)}-J_k^{(r)}\widetilde{\chi}_k^{(r)}J_k^{(r)*},\end{aligned}$$

which proves (111). If $u\in\mathrm{Dom}(\widetilde{A}_k^l)$, Hypotheses (H3) (i) and (ii) imply that $\chi_k^{(r)j}u\in\mathrm{Dom}(\widetilde{A}_k^l)$ and $[A_k^l,\chi_k^{(r)j}]u=0$. Differentiation of the identity (109) w.r.t. θ yields $\tilde{1}_k^{(r)}\widetilde{A}_k^l u=\widetilde{\chi}_k^{(r)}\widetilde{A}_k^l u=\widetilde{A}_k^l\widetilde{\chi}_k^{(r)}u$ and iterating this identity we conclude that

$$\tilde{1}_k^{(r)}\widetilde{A}_k^l u=\widetilde{\chi}_k^{(r)j}\widetilde{A}_k^l u=\widetilde{A}_k^l\widetilde{\chi}_k^{(r)j}u.$$

$\square$

Proof of Theorem 5.2. (i) By construction we have

$$A = \bigoplus_{k=0}^{M} A_k,$$

with $A_k = J_k \widetilde{A}_k J_k^* = 1_k A = A 1_k$, $\mathrm{Dom}(A_k) = \{u \in \mathscr{H}_k \,|\, J_k^* u \in \mathrm{Dom}(\widetilde{A}_k)\}$ and $\widetilde{A}_0 = 0$. We may thus write

$$\mathrm{e}^{\mathrm{i}\theta A} = \bigoplus_{k=0}^{M} \mathrm{e}^{\mathrm{i}\theta A_k}.$$

By using the fact that $J_k^* J_k = \tilde{1}_k$ reduces $\widetilde{A}_k$ (see the proof of Lemma 5.1) we easily show that

$$1_k \mathrm{e}^{\mathrm{i}\theta J_k \widetilde{A}_k J_k^*} 1_k = J_k \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} J_k^*,$$

and thus

$$\mathrm{e}^{\mathrm{i}\theta A} = \bigoplus_{k=0}^{M} J_k \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} J_k^*.$$

By applying (111) and $J_0 \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_0} J_0^* = J_0 J_0^* = 1_0$ we obtain,

$$\mathrm{e}^{\mathrm{i}\theta A_k} = M_k \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} M_k^* + \left(1_k - M_k M_k^*\right).$$

and after summing over k

$$\mathrm{e}^{\mathrm{i}\theta A} = \sum_{k=1}^{M} M_k \mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} M_k^* + \left(I - \sum_{k=1}^{M} M_k M_k^*\right).$$

Since

$$M_k^* \mathrm{Dom}(H) \subset \mathrm{Dom}(\widetilde{H}_k), \qquad M_k \mathrm{Dom}(\widetilde{H}_k) \subset \mathrm{Dom}(H),$$

by Hypothesis (H2) (i), and $\mathrm{e}^{\mathrm{i}\theta \widetilde{A}_k} \mathrm{Dom}(\widetilde{H}_k) \subset \mathrm{Dom}(\widetilde{H}_k)$ by Hypothesis (H3) (iv), we conclude that $\mathrm{Dom}(H)$ is invariant under $\mathrm{e}^{\mathrm{i}\theta A_k}$ and $\mathrm{e}^{\mathrm{i}\theta A}$.

(ii) For $u, v \in \mathrm{Dom}(H) \cap \mathrm{Dom}(A^n)$ such that $A^n u, A^n v \in \mathrm{Dom}(H)$ we have

$$(u, \mathrm{ad}_{A_k}^j(H) v) = \mathrm{i}^j \sum_{l=0}^{j} \binom{j}{l} (-1)^l (J_k \widetilde{A}_k^{j-l} J_k^* u, H J_k \widetilde{A}_k^l J_k^* v). \tag{113}$$

For $l > 0$ we obtain, by using (112)

$$(J_k \widetilde{A}_k^{j-l} J_k^* u, H J_k \widetilde{A}_k^l J_k^* v) = (\widetilde{A}_k^{j-l} J_k^* u, J_k^* H J_k \widetilde{\chi}_k^2 \widetilde{A}_k^l J_k^* v).$$

Hypothesis (H2) (ii) allows us to continue

$$(J_k \widetilde{A}_k^{j-l} J_k^* u, H J_k \widetilde{A}_k^l J_k^* v) = (\widetilde{A}_k^{j-l} J_k^* u, \tilde{1}_k \widetilde{H}_k \widetilde{\chi}_k^2 \widetilde{A}_k^l J_k^* v).$$

By once again invoking (112) and by remarking that

$$\tilde{1}_k \widetilde{A}_k^{j-l} J_k^* u = \widetilde{A}_k^{j-l} \tilde{1}_k J_k^* u = \widetilde{A}_k^{j-l} J_k^* u,$$

we arrive at

$$(J_k \widetilde{A}_k^{j-l} J_k^* u, H J_k \widetilde{A}_k^l J_k^* v) = (\widetilde{A}_k^{j-l} J_k^* u, \widetilde{H}_k \widetilde{A}_k^l J_k^* v).$$

Reapplying (112) gives

$$(J_k \widetilde{A}_k^{j-l} J_k^* u, H J_k \widetilde{A}_k^l J_k^* v) = (\widetilde{A}_k^{j-l} J_k^* u, \widetilde{H}_k \widetilde{\chi}_k^{(2)} \widetilde{A}_k^l \widetilde{\chi}_k J_k^* v),$$

and Identity (108) allows us to write

$$(J_k \widetilde{A}_k^{j-l} J_k^* u, H J_k \widetilde{A}_k^l J_k^* v) = (\widetilde{A}_k^{j-l} J_k^* u, \widetilde{\chi}_k \widetilde{H}_k \widetilde{\chi}_k^{(2)} \widetilde{A}_k^l \chi_k J_k^* v) = (\widetilde{A}_k^{j-l} \widetilde{\chi}_k J_k^* u, \widetilde{H}_k \widetilde{A}_k^l \widetilde{\chi}_k J_k^* v). \tag{114}$$

For $l = 0$ we obtain in an analogous way

$$\begin{aligned}(J_k \widetilde{A}_k^j J_k^* u, H v) &= (H J_k \widetilde{\chi}_k^2 \widetilde{A}_k^j J_k^* u, v) = (J_k \widetilde{H}_k \widetilde{\chi}_k^2 \widetilde{A}_k^j J_k^* u, v) \\ &= (\widetilde{A}_k^j J_k^* u, \widetilde{H}_k J_k^* v) = (\widetilde{A}_k^j \widetilde{\chi}_k J_k^* u, \widetilde{\chi}_k^{(2)} \widetilde{H}_k J_k^* v).\end{aligned}$$

Identity (108) allows us to write

$$(J_k \widetilde{A}_k^j J_k^* u, H v) = (\widetilde{A}_k^j \widetilde{\chi}_k J_k^* u, \widetilde{\chi}_k^{(2)} \widetilde{H}_k \chi_k J_k^* v) = (\widetilde{A}_k^j \widetilde{\chi}_k J_k^* u, \widetilde{H}_k \widetilde{\chi}_k J_k^* v). \tag{115}$$

By gathering (114) and (115) in (113) we conclude that $\mathrm{ad}^j_{A_k}(H) = M_k \mathrm{ad}^j_{\widetilde{A}_k}(\widetilde{H}_k) M_k^*$ and

$$\mathrm{ad}^j_A(H) = \sum_{k=1}^M M_k \mathrm{ad}^j_{\widetilde{A}_k}(\widetilde{H}_k) M_k^*. \tag{116}$$

Hypotheses (H2) (i) and (H3) (v) allow us to conclude that

$$\mathrm{ad}^j_{A_k}(H) \in \mathscr{B}(\mathscr{H}^1_H, \mathscr{H}),$$

for $j \in \{1, \ldots, n\}$ and by consequence that $H \in \mathscr{B}^n_{A_k}(\mathscr{H}^1_H, \mathscr{H})$.

(iii) Since $A = \oplus_{k=1}^M A_k$, Assertion (ii) implies that $H \in \mathscr{B}^n_A(\mathscr{H}^1_H, \mathscr{H})$. By Assertion (i) we may invoke Theorem 4.22 (ii) to conclude that $H \in C^n_{\mathrm{loc}}(A)$.

(iv) Let $E \in \mathbb{R} \setminus \cup_k \Sigma_k$. Hypothesis (H3) stipulates that for $k \in \{1, \ldots, M\}$ there exists $g_k \in C_0^\infty(\mathbb{R})$, $g_k(E) = 1$, $0 \le g_k \le 1$, constants $\theta_k > 0$ and compact operators K_k satisfying

$$g_k(\widetilde{H}_k) \mathrm{i}[\widetilde{H}_k, \widetilde{A}_k] g_k(\widetilde{H}_k) \ge \theta_k g_k(\widetilde{H}_k)^2 + K_k. \tag{117}$$

Since $g_k(E) = 1$, there exists $\delta > 0$ such that $g_k(x) \ge 1/2$ for all $x \in [E-\delta, E+\delta]$ and $k \in \{1, \ldots, M\}$. If $g \in C_0^\infty([E-\delta, E+\delta])$ is such that $g(E) = 1$ and $0 \le g \le 1$ then $h_k = g/g_k \ge 0$ and by multiplying both sides of the inequality (117) by $h_k(\widetilde{H}_k)$ we obtain

$$g(\widetilde{H}_k) \mathrm{i}[\widetilde{H}_k, \widetilde{A}_k] g(\widetilde{H}_k) \ge \theta_k g(\widetilde{H}_k)^2 + K_k',$$

where $K_k' = h_k(\widetilde{H}_k)K_k h_k(\widetilde{H}_k)$ is compact.
Formula (116) and Corollary 5.5 allow us to write

$$\begin{aligned}
g(H)\mathrm{i}[H,A]g(H) &= \sum_{k=1}^{M} g(H)M_k \mathrm{i}[\widetilde{H}_k,\widetilde{A}_k]M_k^* g(H) \\
&= \sum_{k=1}^{M} (M_k g(\widetilde{H}_k)+D_k)\mathrm{i}[\widetilde{H}_k,\widetilde{A}_k](g(\widetilde{H}_k)M_k^*+D_k^*) \\
&= \sum_{k=1}^{M} M_k g(\widetilde{H}_k)\mathrm{i}[\widetilde{H}_k,\widetilde{A}_k]g(\widetilde{H}_k)M_k^* + K,
\end{aligned}$$

where $D_k \equiv D_k^{(1)}(g)$ and K is compact. We thus have

$$g(H)\mathrm{i}[H,A]g(H) \geq \sum_{k=1}^{M} \theta_k M_k g(\widetilde{H}_k)^2 M_k^* + K',$$

where $K' = K + \sum_k M_k K_k' M_k^*$ is again compact. Since

$$M_k g(\widetilde{H}_k)^2 M_k^* = (g(H)M_k - D_k)(M_k^* g(H) - D_k^*),$$

Corollary 5.5 gives us

$$g(H)\mathrm{i}[H,A]g(H) \geq \theta\, g(H)\left(\sum_{k=1}^{M} M_k M_k^*\right) g(H) + K'',$$

where $\theta \equiv \min_k \theta_k > 0$ and K'' is compact. Finally, Hypothesis (H1) (ii) implies

$$\sum_{k=1}^{M} M_k M_k^* = \sum_{k=1}^{M} \chi_k^{(1)2} \geq \sum_{k=1}^{M} 1_k^{(2)} = I - 1_0^{(2)}, \tag{118}$$

and Hypothesis (H2) (vi) allows us to conclude

$$g(H)\mathrm{i}[H,A]g(H) \geq \theta\, g(H)^2 + K''',$$

where $K''' = K'' - \theta g(H) 1_0^{(2)} g(H)$ is compact. H therefore satisfies a Mourre estimate with conjugate operator A for all $E \in \mathbb{R} \setminus \cup_k \Sigma_k$.
Since each Σ_k is closed and countable, so is $\cup_k \Sigma_k$. $J \equiv \mathbb{R} \setminus \cup_k \Sigma_k$ is thus a union of a countable number of open intervals Δ_j. Theorem 4.25 implies that the singular continuous spectrum of H is empty and its eigenvalues can only accumulate at points in $\cup_k \Sigma_k$. This gives that

$$\Sigma_H \equiv \mathrm{Sp}_{\mathrm{pp}}(H) \bigcup \left(\bigcup_{k=1}^{M} \Sigma_k\right),$$

is closed and countable.

Let $E \in \mathbb{R} \setminus \Sigma_H$. The spectrum of H in the neighborhood of E is purely absolutely continuous. Let $f_n \in C_0^\infty(\mathbb{R})$ is a sequence such that $0 \le f_n \le 1$, $\operatorname{supp} f_n \subset [E-1/n, E+1/n]$ and $f_n(E) = 1$. For n large enough $h_n = f_n/g \in C_0^\infty([E-1/n, E+1/n])$ and $0 \le h_n \le 2$. We conclude that

$$\mathrm{s}-\lim_{n\to\infty} h_n(H) = 0,$$

and by consequence

$$\lim_{n\to\infty} \|h_n(H)K''' h_n(H)\| = 0.$$

If n_0 is large enough we have $h_{n_0}(H)K''' h_{n_0}(H) \ge -\theta/4$ and

$$f_{n_0}(H)\mathrm{i}[H,A]f_{n_0}(H) \ge \theta f_{n_0}(H)^2 + h_{n_0}(H)K''' h_{n_0}(H) \ge \theta f_{n_0}(H)^2 - \theta/4.$$

Finally, if $f \in C_0^\infty(\mathbb{R})$ is such that $0 \le f \le 1$, $f(E) = 1$ and $f_{n_0} \ge 1/2$ on $\operatorname{supp} f$ then $\tilde{g} \equiv f f_{n_0} \ge f/2$ and we have

$$\tilde{g}(H)\mathrm{i}[H,A]\tilde{g}(H) \ge \theta \tilde{g}(H)^2 - \theta f(H)^2/4 \ge \theta \tilde{g}(H)^2/4.$$

□

5.4 Scattering theory

In this section we develop some elements of the theory of multi-channel scattering associated with the Hamiltonian H and with the decomposition induced by the identification operators $M_k^{(r)}$.

We shall use the "local smoothness" approach developed by Lavine [La1, La2] on the basis of the theory of "H-smooth" perturbations due to Kato [Ka1] (see Section XIII.7 of [RS4]). This approach has become very effective with the contribution of Mourre theory which allows the construction of locally H-smooth operators from the Mourre estimate ([M2, M3], *c.f.* Corollary 4.26). We shall make intensive use of the abstract two Hilbert space scattering theory as exposed in Section XI.3 of [RS3] (see also [DS]).

5.4.1 Bound states and scattering states

We remark that under Hypotheses (H1), (H2) and (H3) the Hamiltonians of our system have empty singular continuous spectra (by Corollary 5.3). We thus have that $\widetilde{\mathcal{H}}_k = \widetilde{\mathcal{H}}_{k,\mathrm{pp}}(\widetilde{H}_k) \oplus \widetilde{\mathcal{H}}_{k,\mathrm{ac}}(\widetilde{H}_k)$ and $\mathcal{H} = \mathcal{H}_{\mathrm{pp}}(H) \oplus \mathcal{H}_{\mathrm{ac}}(H)$. To simplify notation, we write

$$\widetilde{\mathcal{H}}_k = \widetilde{\mathcal{H}}_{k,\mathrm{pp}} \oplus \widetilde{\mathcal{H}}_{k,\mathrm{ac}}, \qquad \mathcal{H} = \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{ac}},$$

without explicitly mentioning the Hamiltonians.

Adapting ideas of Ruelle, Amrein and Georgescu [R1, AG], we can also decompose these spaces on the basis of the dynamical properties of the states induced by their elements. A vector $u \in \mathcal{H}$ is (improperly) called bound state for $t \to \pm\infty$ if it stays arbitrarily well localized in a neighborhood of the system $\mathfrak{S}$ for $\pm t \ge 0$. More precisely the subspace of bound states for $t \to \pm\infty$ is defined by

$$\mathcal{H}_{\rm b}^{\pm} \equiv \left\{ u \in \mathcal{H} \,\middle|\, \forall \varepsilon > 0 \,\exists R \ge 0 : \sup_{\substack{\pm t \ge 0 \\ r > R}} \|(I - 1_0^{(r)}) \mathrm{e}^{-\mathrm{i}tH} u\| < \epsilon, \right\}.$$

The vector u is a scattering state if it escapes any neighborhood of $\mathfrak{S}$ as $t \to \infty$. The subspace of scattering states is defined by

$$\mathcal{H}_{\rm s}^{\pm} \equiv \left\{ u \in \mathcal{H} \,\middle|\, \forall r \ge 0 : \lim_{t \to \pm\infty} \|1_0^{(r)} \mathrm{e}^{-\mathrm{i}tH} u\| = 0 \right\}.$$

In a similar manner, we define the incoming states of the reservoir $\mathcal{R}_k$ as the states which, when they evolve with the dynamics generated by $\widetilde{H}_k$, are localized in a neighborhood of infinity in the distant past.

$$\widetilde{\mathcal{H}}_k^{\rm in} \equiv \left\{ u \in \widetilde{\mathcal{H}}_k \,\middle|\, \forall r \ge 0 : \lim_{t \to -\infty} \|(I - \tilde{1}_k^{(r)}) \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u\| = 0 \right\}.$$

The outgoing states are also localized in a neighborhood of infinity, but in the distant future

$$\widetilde{\mathcal{H}}_k^{\rm out} \equiv \left\{ u \in \widetilde{\mathcal{H}}_k \,\middle|\, \forall r \ge 0 : \lim_{t \to +\infty} \|(I - \tilde{1}_k^{(r)}) \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u\| = 0 \right\}.$$

The space of all incoming/outgoing states of the full system is

$$\widetilde{\mathcal{H}}^{\rm in/out} \equiv \bigoplus_{k=1}^{M} \widetilde{\mathcal{H}}_k^{\rm in/out}.$$

We easily verify that $\mathcal{H}_{\rm b}^{\pm}$ and $\mathcal{H}_{\rm s}^{\pm}$ are closed subspaces of $\mathcal{H}$ and that $\widetilde{\mathcal{H}}_k^{\rm in}$ and $\widetilde{\mathcal{H}}_k^{\rm out}$ are closed subspaces of $\widetilde{\mathcal{H}}_k$. In particular $\widetilde{\mathcal{H}}^{\rm in/out}$ are Hilbert spaces. The following result shows the relations of these "dynamical" subspaces and the spectral subspaces of the corresponding Hamiltonians. We shall see later in this section that the scattering operator relates the subspaces $\widetilde{\mathcal{H}}^{\rm in}$ and $\widetilde{\mathcal{H}}^{\rm out}$.

Lemma 5.7 *Under the hypotheses (H1), (H2) and (H3) we have*

$$\mathcal{H}_{\rm b}^{+} = \mathcal{H}_{\rm b}^{-} = \mathcal{H}_{\rm pp}, \qquad \mathcal{H}_{\rm s}^{+} = \mathcal{H}_{\rm s}^{-} = \mathcal{H}_{\rm ac},$$

and

$$\widetilde{\mathcal{H}}_k^{\rm in} \subset \widetilde{\mathcal{H}}_{k,\rm ac}, \qquad \widetilde{\mathcal{H}}_k^{\rm out} \subset \widetilde{\mathcal{H}}_{k,\rm ac}.$$

Consequently we shall henceforth write $\mathcal{H}_{\rm b} = \mathcal{H}_{\rm b}^{-} = \mathcal{H}_{\rm b}^{+}$ and $\mathcal{H}_{\rm s} = \mathcal{H}_{\rm s}^{-} = \mathcal{H}_{\rm s}^{+}$.

Proof. If u is an eigenvector of H then

$$\|(I - 1_0^{(r)}) \mathrm{e}^{-\mathrm{i}tH} u\| = \|(I - 1_0^{(r)}) u\|,$$

for all $t \in \mathbb{R}$ and $r \geq 0$. We thus have

$$\|(I - 1_0^{(r)})\mathrm{e}^{-\mathrm{i}tH} u\|^2 = \sum_{k=1}^{M} \|1_k^{(r)} u\|^2,$$

and Hypothesis (H1) (iv) allows us to conclude that

$$\lim_{r\to\infty} \sup_{t\in\mathbb{R}} \|(I - 1_0^{(r)})\mathrm{e}^{-\mathrm{i}tH} u\| = 0,$$

that is to say that $u \in \mathscr{H}_{\mathrm{b}}^- \cap \mathscr{H}_{\mathrm{b}}^+$. Since $\mathscr{H}_{\mathrm{b}}^\pm$ are closed subspaces we get that $\mathscr{H}_{\mathrm{pp}} \subset \mathscr{H}_{\mathrm{b}}^- \cap \mathscr{H}_{\mathrm{b}}^+$.
If $u \in \mathscr{H}_{\mathrm{ac}} \cap \mathrm{Dom}(H)$ we have

$$\|1_0^{(r)} \mathrm{e}^{-\mathrm{i}tH} u\|^2 = \left(\mathrm{e}^{-\mathrm{i}tH} u, 1_0^{(r)} \mathrm{e}^{-\mathrm{i}tH} u\right) \leq \|u\| \, \|1_0^{(r)} (H+\mathrm{i})^{-1} \mathrm{e}^{-\mathrm{i}tH} (H+\mathrm{i}) u\|,$$

and since $1_0^{(r)}(H+\mathrm{i})^{-1}$ is compact by Hypothesis (H2) (vi) and

$$\mathrm{w}-\lim_{t\to\pm\infty} \mathrm{e}^{-\mathrm{i}tH}(H+\mathrm{i})u = 0,$$

by the Riemann-Lebesgue lemma (Lemma 2 of Section XI.3 in [RS3]), we may conclude that

$$\lim_{t\to\pm\infty} \|1_0^{(r)} \mathrm{e}^{-\mathrm{i}tH} u\| = 0,$$

and thus $u \in \mathscr{H}_{\mathrm{s}}^- \cap \mathscr{H}_{\mathrm{s}}^+$. Since $\mathscr{H}_{\mathrm{ac}} \cap \mathrm{Dom}(H)$ is dense in $\mathscr{H}_{\mathrm{ac}}$ and $\mathscr{H}_{\mathrm{s}}^\pm$ are closed, we conclude that $\mathscr{H}_{\mathrm{ac}} \subset \mathscr{H}_{\mathrm{s}}^- \cap \mathscr{H}_{\mathrm{s}}^+$.
We now show that $\mathscr{H}_{\mathrm{s}}^\pm$ and $\mathscr{H}_{\mathrm{b}}^\pm$ are orthogonal to each other. If $u \in \mathscr{H}_{\mathrm{s}}^+$, $v \in \mathscr{H}_{\mathrm{b}}^+$ and $\epsilon > 0$ there exists $R > 0$ such that $\|u\| \, \|(I - 1_0^{(R)})\mathrm{e}^{-\mathrm{i}tH} v\| < \epsilon$ for all $t > 0$. We deduce that

$$\begin{aligned}
|(u,v)| &= |(\mathrm{e}^{-\mathrm{i}tH} u, \mathrm{e}^{-\mathrm{i}tH} v)| \\
&\leq |(\mathrm{e}^{-\mathrm{i}tH} u, (I - 1_0^{(R)})\mathrm{e}^{-\mathrm{i}tH} v)| + |(1_0^{(R)} \mathrm{e}^{-\mathrm{i}tH} u, \mathrm{e}^{-\mathrm{i}tH} v)| \\
&\leq \|u\| \, \|(I - 1_0^{(R)})\mathrm{e}^{-\mathrm{i}tH} v\| + \|1_0^{(R)} \mathrm{e}^{-\mathrm{i}tH} u\| \, \|v\| \\
&\leq \epsilon + \|1_0^{(R)} \mathrm{e}^{-\mathrm{i}tH} u\| \, \|v\|,
\end{aligned}$$

for all $t > 0$, and as $t \to +\infty$ we obtain $|(u,v)| < \epsilon$. Since $\epsilon > 0$ was arbitrary we conclude that $(u,v) = 0$ and consequently that $\mathscr{H}_{\mathrm{s}}^+ \perp \mathscr{H}_{\mathrm{b}}^+$. It is clear that the same argument shows that $\mathscr{H}_{\mathrm{s}}^- \perp \mathscr{H}_{\mathrm{b}}^-$.
We have shown that

$$\begin{aligned}
\mathscr{H} &= \mathscr{H}_{\mathrm{pp}} \oplus \mathscr{H}_{\mathrm{ac}} \subset \mathscr{H}_{\mathrm{b}}^- \oplus \mathscr{H}_{\mathrm{s}}^- \subset \mathscr{H}, \\
\mathscr{H} &= \mathscr{H}_{\mathrm{pp}} \oplus \mathscr{H}_{\mathrm{ac}} \subset \mathscr{H}_{\mathrm{b}}^+ \oplus \mathscr{H}_{\mathrm{s}}^+ \subset \mathscr{H},
\end{aligned}$$

which immediately gives $\mathscr{H}_{\mathrm{ac}} = \mathscr{H}_{\mathrm{s}}^- = \mathscr{H}_{\mathrm{s}}^+$ and $\mathscr{H}_{\mathrm{pp}} = \mathscr{H}_{\mathrm{b}}^- = \mathscr{H}_{\mathrm{b}}^+$.

To show that $\widetilde{\mathscr{H}}_k^{\rm out} \subset \widetilde{\mathscr{H}}_{k,\rm ac}$, it suffices to show that $\widetilde{\mathscr{H}}_{k,\rm pp} \subset \widetilde{\mathscr{H}}_k^{\rm out\perp}$, that is to say that for each eigenvector u of $\widetilde{H}_k$ and for all $v \in \widetilde{\mathscr{H}}_k^{\rm out}$ we have $(u,v) = 0$. If $\widetilde{H}_k u = Eu$ then, for all $r > 0$,

$$\begin{aligned}|(u,v)| &= |(\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}u, \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v)| = |(u, \mathrm{e}^{-\mathrm{i}t(\widetilde{H}_k - E)}v)| \\ &\le |(u, (I - \tilde{1}_k^{(r)})\mathrm{e}^{-\mathrm{i}t(\widetilde{H}_k - E)}v)| + |(\tilde{1}_k^{(r)}u, \mathrm{e}^{-\mathrm{i}t(\widetilde{H}_k - E)}v)| \\ &\le \|u\|\,\|(I - \tilde{1}_k^{(r)})\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v\| + \|\tilde{1}_k^{(r)}u\|\,\|v\|.\end{aligned}$$

By Hypothesis (H1) (iv), for all $\epsilon > 0$, there exists $R > 1$ such that $\|\tilde{1}_k^{(R)}u\|\,\|v\| < \epsilon$. Since

$$\lim_{t\to+\infty} \|u\|\,\|(I - \tilde{1}_k^{(r)})\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v\| = 0,$$

We conclude that $|(u,v)| < \epsilon$ and since $\epsilon > 0$ was arbitrary, we have that $(u,v) = 0$. The last assertion of the lemma is proven in an analogous way. □

5.4.2 The strong topologies of $\mathscr{B}(\mathscr{H})$

Since the strong and strong-$*$ topologies of $\mathscr{B}(\mathscr{H})$ play an essential role in scattering theory, we start by describing some of their important properties (see Section 2.4.1 of [BR1] for a detailed discussion of the various topologies on $\mathscr{B}(\mathscr{H})$).

A net $(B_\iota)_{\iota\in I}$ in $\mathscr{B}(\mathscr{H})$ is strongly convergent if there exists $B \in \mathscr{B}(\mathscr{H})$ such that $\lim_\iota B_\iota u = Bu$. We then write $B = \mathrm{s}-\lim_\iota B_\iota$. If furthermore the family $(B_\iota^*)_{\iota\in I}$ is strongly convergent we say that $(B_\iota)_{\iota\in I}$ is strong-$*$ convergent. In this case we necessarily have that $\mathrm{s}-\lim_\iota B_\iota^* = B^*$, indeed

$$(B^*u, v) = (u, Bv) = \lim_\iota (u, B_\iota v) = \lim_\iota (B_\iota^* u, v) = ((\mathrm{s}-\lim_\iota B_\iota^*)u, v),$$

for all $u, v \in \mathscr{H}$. We then write $\mathrm{s}^*-\lim_\iota B_\iota = B$. Remember however that if $\mathscr{H}$ is infinite dimensional the strong-$*$ topology is strictly finer than the strong topology. The mapping $B \mapsto B^*$ is strong-$*$ continuous but not strongly continuous. The product $\langle A, B\rangle \mapsto AB$ is not strongly continuous. However its restriction to a bounded subset of $\mathscr{B}(\mathscr{H}) \times \mathscr{B}(\mathscr{H})$ is, due to the inequality

$$\|B_\iota C_\iota u - BCu\| \le \|B_\iota\|\,\|(C_\iota - C)u\| + \|(B_\iota - B)Cu\|.$$

If H_1 and H_2 are self-adjoint operators on $\mathscr{H}_1$ and $\mathscr{H}_2$ and if $B \in \mathscr{B}(\mathscr{H}_2, \mathscr{H}_1)$ we denote

$$\Gamma^\pm(H_1, H_2; B) \equiv \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH_1} B \mathrm{e}^{-\mathrm{i}tH_2},$$

when these limits exist. In the sequel we shall use without explicitly mention the following properties of this $\Gamma^\pm$ operation. If $\Gamma^\pm(H_1, H_2; B)$ and $\Gamma^\pm(H_1, H_2; C)$ exist, so does $\Gamma^\pm(H_1, H_2; B + C)$ and

$$\Gamma^\pm(H_1, H_2; B + C) = \Gamma^\pm(H_1, H_2; B) + \Gamma^\pm(H_1, H_2; C).$$

Similarly, if $\Gamma^\pm(H_1, H_2, B)$ and $\Gamma^\pm(H_2, H_3, C)$ exist, so does $\Gamma^\pm(H_1, H_3; BC)$ and

$$\Gamma^\pm(H_1, H_3; BC) = \Gamma^\pm(H_1, H_2; B)\Gamma^\pm(H_2, H_3; C). \tag{119}$$

The limits $\Gamma^{\pm}(H_1, H_2; B)$ and $\Gamma^{\pm}(H_2, H_1; B^*)$ exist simultaneously if and only if

$$\Gamma^{\pm}(H_1, H_2; B) = \mathrm{s}^* - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH_1} B \mathrm{e}^{-\mathrm{i}tH_2},$$

and in this case

$$\Gamma^{\pm}(H_2, H_1; B^*) = \Gamma^{\pm}(H_1, H_2; B)^*.$$

We note that if $\Gamma^{\pm}(H_1, H_2; B)$ exists then

$$\mathrm{s} - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}(s+t)H_1} B \mathrm{e}^{-\mathrm{i}tH_2} = \mathrm{s} - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH_1} B \mathrm{e}^{-\mathrm{i}(t-s)H_2},$$

and thus $\mathrm{e}^{\mathrm{i}sH_1}\Gamma^{\pm}(H_1, H_2; B) = \Gamma^{\pm}(H_1, H_2; B)\mathrm{e}^{\mathrm{i}sH_2}$. We easily conclude that for all measurable functions f, $\Gamma^{\pm}(H_1, H_2; B)\mathrm{Dom}(f(H_2)) \subset \mathrm{Dom}(f(H_1))$ and

$$f(H_1)\Gamma^{\pm}(H_1, H_2; B)u = \Gamma^{\pm}(H_1, H_2; B)f(H_2)u,$$

for all $u \in \mathrm{Dom}(f(H_2))$. In particular,

$$F(H_1 \in I)\Gamma^{\pm}(H_1, H_2; B) = \Gamma^{\pm}(H_1, H_2; B)F(H_2 \in I),$$

for all measurable sets $I \subset \mathbb{R}$. It is then easy to deduce that

$$P_{\mathrm{ac}}(H_2)\Gamma^{\pm}(H_1, H_2; B) = \Gamma^{\pm}(H_1, H_2; B)P_{\mathrm{ac}}(H_1). \tag{120}$$

This relation implies an important extension of the identity (119). Suppose that the limits $\Gamma^{\pm}(H_1, H_2; BP_{\mathrm{ac}}(H_2))$ and $\Gamma^{\pm}(H_2, H_3; CP_{\mathrm{ac}}(H_3))$ exist. We can therefore decompose

$$\begin{aligned}\mathrm{e}^{\mathrm{i}tH_1} BCP_{\mathrm{ac}}(H_3)\mathrm{e}^{-\mathrm{i}tH_3} &= (\mathrm{e}^{\mathrm{i}tH_1} BP_{\mathrm{ac}}(H_2)\mathrm{e}^{-\mathrm{i}tH_2})(\mathrm{e}^{\mathrm{i}tH_2} CP_{\mathrm{ac}}(H_3)\mathrm{e}^{-\mathrm{i}tH_3})\\ &\quad + \mathrm{e}^{\mathrm{i}tH_1} B\mathrm{e}^{-\mathrm{i}tH_2}((I - P_{\mathrm{ac}}(H_2))\mathrm{e}^{\mathrm{i}tH_2} CP_{\mathrm{ac}}(H_3)\mathrm{e}^{-\mathrm{i}tH_3}),\end{aligned}$$

and note that $\mathrm{s} - \lim\limits_{t\to\pm\infty}(I - P_{\mathrm{ac}}(H_2))\mathrm{e}^{\mathrm{i}tH_2} CP_{\mathrm{ac}}(H_3)\mathrm{e}^{-\mathrm{i}tH_3} = 0$ by virtue of (120). We thus obtain

$$\Gamma^{\pm}(H_1, H_3; BCP_{\mathrm{ac}}(H_3)) = \Gamma^{\pm}(H_1, H_2; BP_{\mathrm{ac}}(H_2))\Gamma^{\pm}(H_2, H_3; CP_{\mathrm{ac}}(H_3)).$$

The existence of strong limits $\Gamma^{\pm}(H_1, H_2; J\chi_{\Delta}(H_2))$ can often be proven by combining the propagation estimates with the following result ([Ka1], [La1, La2]); see also Theorem XIII.31 in [RS4] and Chapter 4 of [Y]).

Proposition 5.8 *Let H_1, H_2 be self-adjoint operators on the Hilbert spaces $\mathscr{H}_1$, $\mathscr{H}_2$. Let C_1, C_2 be closed operators on $\mathscr{H}_1$, $\mathscr{H}_2$. Finally, let $J, B \in \mathscr{B}(\mathscr{H}_2, \mathscr{H}_1)$ and $\Delta \subset \mathbb{R}$ be such that*

(i) $\mathrm{Dom}(H_i) \subset \mathrm{Dom}(C_i)$ *and C_i is H_i-bounded for $i = 1, 2$.*

(ii) For all $u_i \in \mathrm{Dom}(H_i)$,

$$(H_1u_1, Ju_2) - (u_1, JH_2u_2) = (C_1u_1, BC_2u_2).$$

(iii) For all $u_i \in \mathcal{H}_i$ and for almost all $t \in \mathbb{R}$, $\mathrm{e}^{-\mathrm{i}tH_i}\chi_\Delta(H_i)u_i \in \mathrm{Dom}(C_i)$ and there exist constants c_1, c_2 such that

$$\int_{-\infty}^{\infty} \|C_i \mathrm{e}^{-\mathrm{i}tH_i}\chi_\Delta(H_i)u_i\|^2\,\mathrm{d}t \le c_i\,\|u_i\|^2.$$

Then $\Gamma^\pm(H_1,H_2;J\chi_\Delta(H_2))$ and $\Gamma^\pm(H_2,H_1;J^*\chi_\Delta(H_1))$ exist. Furthermore

(a) $\Gamma^\pm(H_2,H_1;J^*\chi_\Delta(H_1)) = \Gamma^\pm(H_1,H_2;J\chi_\Delta(H_2))^*$.

(b) $\Gamma^\pm(H_1,H_2;J\chi_\Delta(H_2))\Gamma^\pm(H_1,H_2;J\chi_\Delta(H_2))^* = \Gamma^\pm(H_1,H_1;JJ^*\chi_\Delta(H_1))$.

(c) $\Gamma^\pm(H_2,H_1;J^*\chi_\Delta(H_1))\Gamma^\pm(H_2,H_1;J^*\chi_\Delta(H_1))^* = \Gamma^\pm(H_2,H_2;J^*J\chi_\Delta(H_2))$.

Remark. An operator C_1 satisfying the condition (iii) is called locally H_1-smooth on Δ or simply H_1-smooth if $\Delta = \mathbb{R}$ (see Section XIII.7 of [RS4]).

Proof. We first show that $\Gamma^\pm(H_1,H_2;\chi_\Delta(H_1)J\chi_\Delta(H_2))$ exists. With $u_i \in \mathrm{Dom}(H_i)$ we can write

$$(u_1,u_2(t')) - (u_1,u_2(t)) = \mathrm{i}\int_t^{t'} (C_1\mathrm{e}^{-\mathrm{i}sH_1}\chi_\Delta(H_1)u_1, BC_2\mathrm{e}^{-\mathrm{i}sH_2}\chi_\Delta(H_2)u_2)\,\mathrm{d}s,$$

where $u_2(t) \equiv \mathrm{e}^{\mathrm{i}tH_1}\chi_\Delta(H_1)J\chi_\Delta(H_2)\mathrm{e}^{-\mathrm{i}tH_2}u_2$. We then have

$$\begin{aligned}
|(u_1,u_2(t')-u_2(t))| &\le \|B\|\int_t^{t'} \|C_1\mathrm{e}^{-\mathrm{i}sH_1}\chi_\Delta(H_1)u_1\|\,\|C_2\mathrm{e}^{-\mathrm{i}sH_2}\chi_\Delta(H_2)u_2\|\,\mathrm{d}s\\
&\le \|B\|\left(\int_t^{t'} \|C_1\mathrm{e}^{-\mathrm{i}sH_1}\chi_\Delta(H_1)u_1\|^2\,\mathrm{d}s\right)^{1/2}\left(\int_t^{t'} \|C_2\mathrm{e}^{-\mathrm{i}sH_2}\chi_\Delta(H_2)u_2\|^2\,\mathrm{d}s\right)^{1/2}\\
&\le c_1^{1/2}\|B\|\,\|u_1\|\left(\int_t^{t'} \|C_2\mathrm{e}^{-\mathrm{i}sH_2}\chi_\Delta(H_2)u_2\|^2\,\mathrm{d}s\right)^{1/2},
\end{aligned}$$

and thus

$$\|u_2(t')-u_2(t)\| \le c_1^{1/2}\|B\|\left(\int_t^{t'} \|C_2\mathrm{e}^{-\mathrm{i}sH_2}\chi_\Delta(H_2)u_2\|^2\,\mathrm{d}s\right)^{1/2},$$

which allows us to conclude that $u_2(t)$ converges when $t \to \pm\infty$. This extends by continuity to all $u_2 \in \mathcal{H}_2$.

We now prove that $\Gamma^\pm(H_1,H_2;\chi_{\Delta^c}(H_1))J\chi_\Delta(H_2)) = 0$. To do this it suffices to show that

$$\Gamma^\pm(H_1,H_2;\chi_{\Delta^c}(H_1)J\chi_{\Delta'}(H_2)) = 0,$$

for all compact intervals $\Delta' \subset \Delta$. Let $g \in C_0^\infty(\Delta)$ such that $0 \le g \le 1$ and $g = 1$ on Δ'. For $u_2 \in \mathcal{H}_2$, let $u_2(t) \equiv \mathrm{e}^{\mathrm{i}tH_1}\chi_{\Delta^c}(H_1)J\chi_{\Delta'}(H_2)\mathrm{e}^{-\mathrm{i}tH_2}u_2$, so that

$$u_2(t) = \mathrm{e}^{\mathrm{i}tH_1}\chi_{\Delta^c}(H_1)(Jg(H_2)-g(H_1)J)\mathrm{e}^{-\mathrm{i}tH_2}\chi_{\Delta'}(H_2)u_2.$$

By setting $R_i(z) \equiv (H_i - z)^{-1}$, property (ii) allows us to write, for $u_1 \in \mathscr{H}_1$,

$$\begin{aligned}&(\mathrm{e}^{-\mathrm{i}tH_1}\chi_{\Delta^c}(H_1)u_1, (JR_2(z) - R_1(z)J)\mathrm{e}^{-\mathrm{i}tH_2}\chi_{\Delta'}(H_2)u_2)\\ &= (C_1R_1(\overline{z})\mathrm{e}^{-\mathrm{i}tH_1}\chi_{\Delta^c}(H_1)u_1, BC_2R_2(z)\mathrm{e}^{-\mathrm{i}tH_2}\chi_{\Delta'}(H_2)u_2),\end{aligned}$$

and the Helffer-Sjöstrand formula gives

$$(u_1, u_2(t)) = \int_{\mathbb{C}} \overline{\partial}\tilde{g}\,(C_1R_1(\overline{z})\mathrm{e}^{-\mathrm{i}tH_1}\chi_{\Delta^c}(H_1)u_1, BC_2R_2(z)\mathrm{e}^{-\mathrm{i}tH_2}\chi_{\Delta'}(H_2)u_2)\frac{\mathrm{d}z\wedge\mathrm{d}\overline{z}}{2\pi},$$

where $\tilde{g}$ is an almost-analytic extension of g. We therefore obtain the following estimate

$$\begin{aligned}|(u_1, u_2(t))| \le \|u_1\|\,\|B\| &\left(\int_{\mathbb{C}} |\overline{\partial}\tilde{g}|\,\|C_1R_1(\overline{z})\|^2\frac{\mathrm{d}z\wedge\mathrm{d}\overline{z}}{2\pi}\right)^{1/2}\times\\ &\left(\int_{\mathbb{C}} |\overline{\partial}\tilde{g}|\,\|C_2\mathrm{e}^{-\mathrm{i}tH_2}R_2(z)\chi_{\Delta'}(H_2)u_2\|^2\frac{\mathrm{d}z\wedge\mathrm{d}\overline{z}}{2\pi}\right)^{1/2}.\end{aligned}$$

Since $C_1R_1(\overline{z}) = C_1R_1(\mathrm{i})(I + (\overline{z} - \mathrm{i})R_1(\overline{z}))$, property (i) allows us to write $\|C_1R_1(\overline{z})\| \le c\,|\mathrm{Im}z|^{-1}$ for a constant c and $z \in \operatorname{supp}\tilde{g}$. Therefore there exists a constant c' such that

$$\|u_2(t)\| \le c'\left(\int_{\mathbb{C}} |\overline{\partial}\tilde{g}|\,\|C_2\mathrm{e}^{-\mathrm{i}tH_2}R_2(z)\chi_{\Delta'}(H_2)u_2\|^2\frac{\mathrm{d}z\wedge\mathrm{d}\overline{z}}{2\pi}\right)^{1/2}.$$

We denote by $f(z,t)$ the integrand on the right hand side of this inequality. Property (i) and an appropriate choice of almost-analytic extension $\tilde{g}$ (recall Estimate (5)) show that for a constant c'' we have

$$0 \le f(z,t) \le c''\frac{|\overline{\partial}\tilde{g}|}{|\mathrm{Im}z|^2} \in L^1(\mathbb{C}, \mathrm{d}z\wedge\mathrm{d}\overline{z}).$$

It is therefore enough for us to show that $\lim_{t\to\pm\infty} f(z,t) = 0$ for all $z \in \mathbb{C}\setminus\mathbb{R}$ to be able to conclude. Property (iii) shows that for such a z we have $f \in L^1(\mathbb{R}, \mathrm{d}t)$. Furthermore, f is differentiable and

$$\partial_t f(z,t) = 2|\overline{\partial}\tilde{g}|\mathrm{Im}(C_2\mathrm{e}^{-\mathrm{i}tH_2}R_2(z)\chi_{\Delta'}(H_2)u_2, C_2\mathrm{e}^{-\mathrm{i}tH_2}R_2(z)H_2\chi_{\Delta'}(H_2)u_2),$$

shows that $|\partial_t f(z,t)| \in L^1(\mathbb{R}, \mathrm{d}t)$. The required property follows immediately.

So we have shown that

$$\begin{aligned}\Gamma^{\pm}(H_1, H_2; J\chi_\Delta(H_2)) &= \Gamma^{\pm}(H_1, H_2; \chi_\Delta(H_1)J\chi_\Delta(H_2)) + \Gamma^{\pm}(H_1, H_2; \chi_{\Delta^c}(H_1)J\chi_\Delta(H_2))\\ &= \Gamma^{\pm}(H_1, H_2; \chi_\Delta(H_1)J\chi_\Delta(H_2)).\end{aligned}$$

The existence of the strong limits $\Gamma^{\pm}(H_2, H_1; J^*\chi_\Delta(H_1))$ is therefore a consequence of the $1 \leftrightarrow 2$ symmetry of our hypotheses.

Assertion (a) is a consequence of the strong-$*$ convergence as we explicitly mentioned above. Assertion (b) follows from the identity

$$\begin{aligned}\mathrm{e}^{\mathrm{i}tH_1}JJ^*\chi_\Delta(H_1)\mathrm{e}^{-\mathrm{i}tH_1} &= \mathrm{e}^{\mathrm{i}tH_1}J\chi_\Delta(H_2)\mathrm{e}^{-\mathrm{i}tH_2}\mathrm{e}^{\mathrm{i}tH_2}J^*\chi_\Delta(H_1)\mathrm{e}^{-\mathrm{i}tH_1}\\ &+ \mathrm{e}^{\mathrm{i}tH_1}J\mathrm{e}^{-\mathrm{i}tH_2}\chi_{\Delta^c}(H_2)\mathrm{e}^{\mathrm{i}tH_2}J^*\chi_\Delta(H_1)\mathrm{e}^{-\mathrm{i}tH_1},\end{aligned}$$

and the fact that $\chi_{\Delta^c}(H_2)\Gamma^{\pm}(H_2,H_1;J^*\chi_{\Delta}(H_1))=0$. Assertion (c) is proven in the same way. □

The following notions shall be useful to us.

Definition 5.9 *Let H be a self-adjoint operator on the Hilbert space $\mathcal{H}$.*

(i) An operator $B\in\mathcal{B}(\mathcal{H})$ is called an asymptotic projection for H if the limits $\Gamma^{\pm}(H,H;B)$ exist and define orthogonal projections

(ii) Two operators $B,C\in\mathcal{B}(\mathcal{H})$ are said to be asymptotically H-equivalent if $\Gamma^{\pm}(H,H;B-C)=0$.

5.4.3 Møller operators

To allow us to briefly describe the basic ideas behind multi-channel scattering theory, we start with a result establishing the existence of asymptotic projection operators for the reference dynamics in the reservoirs. We defer its proof to the end of the section.

Lemma 5.10 *Under hypotheses (H1), (H2), and (H3), for $k\in\{1,\dots,M\}$, $\tilde{1}_k P_{\rm ac}(\widetilde{H}_k)$ is an asymptotic projection for $\widetilde{H}_k$. Furthermore, for $r\geq 1$ the operators $M_k^{(r)*}M_k^{(r)}P_{\rm ac}(\widetilde{H}_k)$, $\tilde{1}_k^{(r)}P_{\rm ac}(\widetilde{H}_k)$ and $\tilde{\chi}_k^{(r)}P_{\rm ac}(\widetilde{H}_k)$ are $\widetilde{H}_k$-equivalent to $\tilde{1}_kP_{\rm ac}(\widetilde{H}_k)$ and*

$$\widetilde{P}_k^{\rm in/out}\equiv\Gamma^{-/+}(\widetilde{H}_k,\widetilde{H}_k;1_kP_{\rm ac}(\widetilde{H}_k)),$$

are the orthogonal projections onto $\widetilde{\mathcal{H}}_k^{\rm in/out}$.

In the sequel, we shall sometimes refer to $\widetilde{P}_k^{\rm in/out}$ as $\widetilde{P}_k^{-/+}$.

Working hypothesis: When it evolves under the dynamics generated by the Hamiltonian H a scattering state of the complete system, $u\in\mathcal{H}_{\rm s}$, behaves asymptotically, when $t\to-\infty$, as a state $u^{\rm in}\in\widetilde{\mathcal{H}}^{\rm in}$ under the dynamics generated by $\widetilde{H}=\oplus_k\widetilde{H}_k$. Similarly, when $t\to+\infty$, it behaves like a state $u^{\rm out}\in\widetilde{\mathcal{H}}^{\rm out}$. More precisely, we have

$$\mathrm{e}^{-\mathrm{i}tH}u\sim\left\{\begin{array}{ll}\sum_{k=1}^M J_k\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}u_k^{\rm in} & \text{for } t\to-\infty,\\ \sum_{k=1}^M J_k\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}u_k^{\rm out} & \text{for } t\to+\infty,\end{array}\right. \tag{121}$$

where $u_k^{\rm in/out}$ denote the projections of $u^{\rm in/out}$ in $\widetilde{\mathcal{H}}_k$ and $f(t)\sim g(t)$ means that $\lim(f(t)-g(t))=0$.

With this hypothesis, we shall construct the central object of scattering theory: the scattering matrix

$$\begin{array}{rcl}S:\widetilde{\mathcal{H}}^{\rm in} & \to & \widetilde{\mathcal{H}}^{\rm out}\\ u^{\rm in} & \mapsto & u^{\rm out}.\end{array}$$

which transforms the incoming asymptote $u^{\rm in} \in \widetilde{\mathscr{H}}^{\rm in}$ into the outgoing asymptote $u^{\rm out} \in \widetilde{\mathscr{H}}^{\rm out}$. This map can be calculated in two steps. We first determine the Møller operators which, to an incoming/outgoing asymptote $u^{\rm in/out}$ associate the scattering state u. These transformations are easily obtained from (121)

$$\Omega^- : u^{\rm in} \mapsto u = \lim_{t\to-\infty} \sum_{k=1}^{M} \mathrm{e}^{\mathrm{i}tH} J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm in},$$
$$\Omega^+ : u^{\rm out} \mapsto u = \lim_{t\to+\infty} \sum_{k=1}^{M} \mathrm{e}^{\mathrm{i}tH} J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm out}.$$

If the Møller operators so defined exist, they are isometric. Indeed Hypothesis (H1) (iii) allows us to write

$$\begin{aligned}\|\Omega^+ u^{\rm out}\|^2 &= \lim_{t\to+\infty} \left\| \sum_{k=1}^{M} J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm out} \right\|^2 \\ &= \sum_{k=1}^{M} \lim_{t\to+\infty} (\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm out}, \tilde{1}_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm out}) \\ &= \sum_{k=1}^{M} \left(\|u_k^{\rm out}\|^2 - \lim_{t\to+\infty} \|(I-\tilde{1}_k)\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm out}\|^2 \right) \\ &= \sum_{k=1}^{M} \|u_k^{\rm out}\|^2 = \|u^{\rm out}\|^2.\end{aligned}$$

It is clear that an identical argument shows that Ω^- is also isometric. In particular the Møller operators are injective, their images $\operatorname{Ran}\Omega^\pm$ are closed, and $(\Omega^\pm)^{-1} = \Omega^{\pm *} : \operatorname{Ran}\Omega^\pm \to \widetilde{\mathscr{H}}^{\rm in/out}$ are isometries. It is thus possible to define $S = \Omega^{+*}\Omega^-$ if $\operatorname{Ran}\Omega^- = \operatorname{Ran}\Omega^+$. In this case, we say that the Møller operators are *weakly asymptotically complete* and we have

$$S^* S = \Omega^{-*}\Omega^+\Omega^{+*}\Omega^- = \Omega^{-*}\Omega^- = I_{\widetilde{\mathscr{H}}^{\rm in}},$$
$$SS^* = \Omega^{+*}\Omega^-\Omega^{-*}\Omega^+ = \Omega^{+*}\Omega^+ = I_{\widetilde{\mathscr{H}}^{\rm out}},$$

that is to say that the scattering matrix is unitary.

We return now to our working hypothesis. Suppose that the Møller operators exist and are weakly asymptotically complete. If $u \in \operatorname{Ran}\Omega^\pm$ then $u = \Omega^\pm u^{\rm in/out}$ and we have

$$0 = \|u - \Omega^\pm u^{\rm in/out}\| = \lim_{t\to\pm\infty} \left\| \mathrm{e}^{-\mathrm{i}tH} u - \sum_{j=1}^{M} J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\rm in/out} \right\|.$$

A posteriori, our working hypothesis is thus verified for all $u \in \operatorname{Ran}\Omega^\pm$. However, if $\operatorname{Ran}\Omega^\pm \neq \mathscr{H}_{\rm s}$ there exists $u \in \mathscr{H}_{\rm s}$ such that $0 \neq u \perp \operatorname{Ran}\Omega^\pm$. In this case (121) and Lemma 5.10 imply that, for all $v^{\mathrm{in/out}} \in \widetilde{\mathscr{H}}^{\mathrm{in/out}}$,

$$
\begin{aligned}
0 = (u, \Omega^{\pm} v^{\mathrm{in/out}}) &= \sum_{k=1}^{M} \lim_{t\to\pm\infty} (\mathrm{e}^{-\mathrm{i}tH} u, J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} v_k^{\mathrm{in/out}}) \\
&= \sum_{k=1}^{M} \lim_{t\to\pm\infty} (J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u_k^{\mathrm{in/out}}, J_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} v_k^{\mathrm{in/out}}) \\
&= \sum_{k=1}^{M} \lim_{t\to\pm\infty} (u_k^{\mathrm{in/out}}, \mathrm{e}^{\mathrm{i}t\widetilde{H}_k} \tilde{1}_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} v_k^{\mathrm{in/out}}) \\
&= \sum_{k=1}^{M} (u_k^{\mathrm{in/out}}, \widetilde{P}_k^{\mathrm{in/out}} v_k^{\mathrm{in/out}}) \\
&= (u^{\mathrm{in/out}}, v^{\mathrm{in/out}}).
\end{aligned}
$$

We obtain from this that $u^{\mathrm{in/out}} = 0$ which implies that $u = 0$, a contradiction. The weak asymptotic completeness is thus not sufficient to assure the validity of (121). It is necessary to also require $\mathscr{H}_{\mathrm{s}} = \operatorname{Ran}\Omega^{-} = \operatorname{Ran}\Omega^{+}$. When this condition is satisfied, we say that the Møller operators are *asymptotically complete.*

Remark 5.2 In our case, because of Lemma 5.7, asymptotic completeness is equivalent to the condition $\operatorname{Ran}\Omega^{-} = \operatorname{Ran}\Omega^{+} = \mathscr{H}_{\mathrm{b}}^{\perp}$. However this last condition is generally stronger than $\operatorname{Ran}\Omega^{-} = \operatorname{Ran}\Omega^{+} = \mathscr{H}_{\mathrm{s}}$. The Møller operators are called complete if $\operatorname{Ran}\Omega^{-} = \operatorname{Ran}\Omega^{+} = \mathscr{H}_{\mathrm{b}}^{\perp}$.

Proposition 5.11 *Under Hypotheses (H1), (H2), and (H3) the partial Møller operators*

$$
\Omega_k^{\pm} \equiv \Gamma^{\pm}(H, \widetilde{H}_k; J_k^{(r)} P_{\mathrm{ac}}(\widetilde{H}_k)),
$$

exist, do not depend on choice of $r > 0$, and satisfy

$$
\Omega_k^{\pm *} \Omega_l^{\pm} = \delta_{kl} \widetilde{P}_k^{\pm}, \qquad \sum_{k=1}^{M} \Omega_k^{\pm} \Omega_k^{\pm *} = P_{\mathrm{ac}}(H).
$$

In particular, the Møller operators $\Omega^{\pm} = \oplus_{k=1}^{M} \Omega_k^{\pm} : \oplus_{k=1}^{M} \widetilde{\mathscr{H}}_k \to \mathscr{H}$ are complete:

$$
\operatorname{Ran}\Omega^{-} = \operatorname{Ran}\Omega^{+} = \mathscr{H}_{\mathrm{s}} = \mathscr{H}_{\mathrm{b}}^{\perp} = \mathscr{H}_{\mathrm{ac}}.
$$

Corollary 5.12 *Under the hypotheses (H1), (H2), and (H3) the operators $1_k^{(r)} P_{\mathrm{ac}}(H)$ are asymptotic projections for H and*

$$
P_k^{\pm} \equiv \Gamma^{\pm}(H, H; 1_k^{(r)} P_{\mathrm{ac}}(H)) = \Omega_k^{\pm} \Omega_k^{\pm *} = \Omega^{\pm} \widetilde{P}_k^{\pm} \Omega^{\pm *},
$$

for all $r \geq 0$ Furthermore $P_k^{\pm} P_l^{\pm} = \delta_{kl} P_k^{\pm}$, $\sum_{k=1}^{M} P_k^{\pm} = P_{\mathrm{ac}}(H)$ and

$$
\operatorname{Ran} P_k^{\pm} = \operatorname{Ran}\Omega_k^{\pm} = \{u \in \mathscr{H}_{\mathrm{s}} \mid \lim_{t\to\pm\infty} \|(I - 1_k^{(r)}) \mathrm{e}^{-\mathrm{i}tH} u\| = 0, \textit{ for all } r \geq 0\}.
$$

Remarks. 1. By setting $\widetilde{H} \equiv \oplus_{k=1}^{M} \widetilde{H}_k$ and

$$\begin{array}{rccc} J: & \oplus_{k=1}^{M} \widetilde{\mathcal{H}}_k & \to & \mathcal{H} \\ & (u_1, \dots, u_M) & \mapsto & \sum_{k=1}^{M} J_k u_k \end{array}$$

we may write

$$\Omega^{\pm} = \Gamma^{\pm}(H, \widetilde{H}; J P_{\rm ac}(\widetilde{H})).$$

We thus have the intertwining relation

$$\Omega^{\pm} f(\widetilde{H}) = f(H)\Omega^{\pm}.$$

We also note the identities $\Omega^{\pm}\widetilde{P}_k^{\pm} = \Omega_k^{\pm} = P_k^{\pm}\Omega^{\pm}$ and the intertwining relations for the partial Møller operators

$$\Omega_k^{\pm} f(\widetilde{H}_k) = f(H)\Omega_k^{\pm}.$$

2. The scattering matrix $S = \Omega^{+*}\Omega^{-} : \widetilde{\mathcal{H}}^{\rm in} \to \widetilde{\mathcal{H}}^{\rm out}$ is unitary. The decompositions $\widetilde{\mathcal{H}}^{\rm in} = \oplus_{k=1}^{M} \widetilde{\mathcal{H}}_k^{\rm in}$ and $\widetilde{\mathcal{H}}^{\rm out} = \oplus_{k=1}^{M} \widetilde{\mathcal{H}}_k^{\rm out}$ allow us to write $S = (S_{kj})$ and $S^* = (S_{kj}^*)$ with

$$\begin{aligned} S_{kj} &= \Omega_k^{+*}\Omega_j^{-} : \widetilde{\mathcal{H}}_j^{\rm in} \to \widetilde{\mathcal{H}}_k^{\rm out}, \\ S_{kj}^* = (S_{jk})^* &= \Omega_k^{-*}\Omega_j^{+} : \widetilde{\mathcal{H}}_j^{\rm out} \to \widetilde{\mathcal{H}}_k^{\rm in}. \end{aligned}$$

The unitarity of S is thus written as

$$\sum_{j=1}^{M} S_{kj}^* S_{jl} = \delta_{kl}\, I_{\widetilde{\mathcal{H}}_k^{\rm in}}, \qquad \sum_{j=1}^{M} S_{kj} S_{jl}^* = \delta_{kl}\, I_{\widetilde{\mathcal{H}}_k^{\rm out}}.$$

For the proof of these results we shall use the following lemma.

Lemma 5.13 *Under Hypotheses (H1), (H2) and (H3) the following assertions hold.*

(i) For all $k \in \{1, \dots, M\}$ and $g \in C_0^\infty(\mathbb{R})$, the quadratic form

$$\widetilde{\xi}_{k,g}(u, v) = (g(\widetilde{H}_k)(\widetilde{A}_k^2 + 1)u, \mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k]g(\widetilde{H}_k)(\widetilde{A}_k^2 + 1)v),$$

defined on $\mathrm{Dom}(\widetilde{A}_k^2) \times \mathrm{Dom}(\widetilde{A}_k^2)$ is bounded. We denote by $\widetilde{\Xi}_{k,g} \in \mathcal{B}(\mathcal{H})$ the operator it defines.

(ii) For all $k \in \{1, \dots, M\}$ and $g \in C_0^\infty(\mathbb{R})$, the quadratic form

$$\xi_{k,g}(u, v) = (g(H)(A^2 + 1)u, J_k \mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k]g(\widetilde{H}_k)(\widetilde{A}_k^2 + 1)v),$$

defined on $\mathrm{Dom}(A^2) \times \mathrm{Dom}(\widetilde{A}_k^2)$ is bounded and $\Xi_{k,g} \in \mathcal{B}(\mathcal{H})$ denotes the associated operator.

Proof. (i) By invoking Theorem 4.22 and Definition 4.11, we remark that Hypothesis (H3) (v) implies that $[\widetilde{A}_k, g(\widetilde{H}_k)]$ is bounded. Furthermore, Lemma 4.2 ensures that $g(\widetilde{H}_k)\mathrm{Dom}(\widetilde{A}_k) \subset \mathrm{Dom}(\widetilde{A}_k)$. We may thus write, for all $u, v \in \mathrm{Dom}(\widetilde{A}_k)$,

$$\widetilde{\xi}_{k,g}(u,v) = ((g(\widetilde{H}_k) + \widetilde{A}_k g(\widetilde{H}_k)\widetilde{A}_k - [\widetilde{A}_k, g(\widetilde{H}_k)]\widetilde{A}_k)u, \mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k]g(\widetilde{H}_k)(\widetilde{A}_k^2+1)v).$$

By a repeated use of the identities (108) and (112), we obtain

$$\begin{aligned}
(\widetilde{A}_k u, [\widetilde{H}_k, \widetilde{\chi}_k]v) &= (\widetilde{A}_k u, \widetilde{H}_k\widetilde{\chi}_k^{(1)}v - \widetilde{\chi}_k^{(1)}\widetilde{H}_k v)\\
&= (\widetilde{A}_k u, \widetilde{\chi}_k^{(0)}\widetilde{H}_k\widetilde{\chi}_k^{(1)}v - \widetilde{\chi}_k^{(1)}\widetilde{H}_k v)\\
&= (\widetilde{\chi}_k^{(0)}\widetilde{A}_k u, \widetilde{H}_k\widetilde{\chi}_k^{(1)}v) - (\widetilde{A}_k u, \widetilde{\chi}_k^{(1)}\widetilde{H}_k v)\\
&= (\widetilde{\chi}_k^{(2)}\widetilde{A}_k u, \widetilde{H}_k\widetilde{\chi}_k^{(1)}v) - (\widetilde{A}_k u, \widetilde{\chi}_k^{(1)}\widetilde{H}_k v)\\
&= (\widetilde{A}_k u, \widetilde{\chi}_k^{(2)}\widetilde{H}_k\widetilde{\chi}_k^{(1)}v - \widetilde{\chi}_k^{(1)}\widetilde{H}_k v)\\
&= (\widetilde{A}_k u, \widetilde{\chi}_k^{(2)}\widetilde{H}_k v - \widetilde{\chi}_k^{(1)}\widetilde{H}_k v)\\
&= ((\widetilde{\chi}_k^{(2)} - \widetilde{\chi}_k^{(1)})\widetilde{A}_k u, \widetilde{H}_k v)\\
&= 0,
\end{aligned} \tag{122}$$

for all $u \in \mathrm{Dom}(\widetilde{A}_k)$ and $v \in \mathrm{Dom}(\widetilde{H}_k)$. We may conclude that

$$\widetilde{\xi}_{k,g}(u,v) = ((g(\widetilde{H}_k) - [\widetilde{A}_k, g(\widetilde{H}_k)]\widetilde{A}_k)u, \mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k]g(\widetilde{H}_k)(\widetilde{A}_k^2+1)v).$$

The same reasoning shows us that Hypothesis (H3) (v) also implies that $[\widetilde{A}_k, [\widetilde{A}_k, g(\widetilde{H}_k)]]$ is bounded and that $[\widetilde{A}_k, g(\widetilde{H}_k)]\mathrm{Dom}(\widetilde{A}_k) \subset \mathrm{Dom}(\widetilde{A}_k)$. From this we get, with the help of the identity (122),

$$\widetilde{\xi}_{k,g}(u,v) = ((g(\widetilde{H}_k) + [\widetilde{A}_k, [\widetilde{A}_k, g(\widetilde{H}_k)]])u, \mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k]g(\widetilde{H}_k)(\widetilde{A}_k^2+1)v).$$

By using the expansion

$$[\widetilde{A}_k, [\widetilde{A}_k, \widetilde{R}_k(z)]] = 2\widetilde{R}_k(z)[\widetilde{A}_k, \widetilde{H}_k]\widetilde{R}_k(z)[\widetilde{A}_k, \widetilde{H}_k]\widetilde{R}_k(z) - \widetilde{R}_k(z)[\widetilde{A}_k, [\widetilde{A}_k, \widetilde{H}_k]]\widetilde{R}_k(z),$$

Hypothesis (H3) (v) and the Helffer-Sjöstrand formula, we easily show that $[\widetilde{A}_k[\widetilde{A}_k, g(\widetilde{H}_k)]] \in \mathscr{B}(\mathscr{H}_k, \mathscr{H}_k^1)$. Since $[\widetilde{H}_k, \widetilde{\chi}_k] \in \mathscr{B}(\mathscr{H}_k^1, \mathscr{H}_k)$ we may write

$$\widetilde{\xi}_{k,g}(u,v) = (\mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k](g(\widetilde{H}_k) + [\widetilde{A}_k, [\widetilde{A}_k, g(\widetilde{H}_k)]])u, g(\widetilde{H}_k)(\widetilde{A}_k^2+1)v).$$

By repeating our argument on the second factor of the scalar product on the right hand side of this identity we show that

$$\widetilde{\xi}_{k,g}(u,v) = (\mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k](g(\widetilde{H}_k) + [\widetilde{A}_k, [\widetilde{A}_k, g(\widetilde{H}_k)]])u, (g(\widetilde{H}_k) + [\widetilde{A}_k, [\widetilde{A}_k, g(\widetilde{H}_k)]])v),$$

which allows us to conclude that

$$|\widetilde{\xi}_{k,g}(u,v)| \leq \|[\widetilde{H}_k, \widetilde{\chi}_k]\|_{\mathscr{B}(\mathscr{H}_k^1, \mathscr{H}_k)} \|g(\widetilde{H}_k) + [\widetilde{A}_k[\widetilde{A}_k, g(\widetilde{H}_k)]]\|^2_{\mathscr{B}(\mathscr{H}_k, \mathscr{H}_k^1)} \|u\|\,\|v\|.$$

(ii) The second assertion is proven in a very similar way. It suffices to note that, for all $u \in \mathrm{Dom}(A)$ and $v \in \mathrm{Dom}(\widetilde{H}_k)$, we have $J_k^* u \in \mathrm{Dom}(\widetilde{A}_k)$ (see Lemma 5.1) and thus, by the identity (122),

$$\begin{aligned}(Au, J_k[\widetilde{H}_k, \widetilde{\chi}_k]v) &= (Au, 1_k J_k[\widetilde{H}_k, \widetilde{\chi}_k]v) = (1_k Au, J_k[\widetilde{H}_k, \widetilde{\chi}_k]v)\\ &= (J_k\widetilde{A}_k J_k^* u, J_k[\widetilde{H}_k, \widetilde{\chi}_k]v)\\ &= (\widetilde{A}_k J_k^* u, [\widetilde{H}_k, \widetilde{\chi}_k]v)\\ &= 0.\end{aligned} \tag{123}$$

By invoking Theorem 5.2 (ii) we obtain, for all $u \in \mathrm{Dom}(A^2)$ and for all $v \in \mathrm{Dom}(\widetilde{A}_k)$,

$$\xi_{k,g}(u,v) = ((g(H) + [A,[A,g(H)]])u, J_k\mathrm{i}[\widetilde{H}_k, \widetilde{\chi}_k](g(\widetilde{H}_k) + [\widetilde{A}_k[\widetilde{A}_k, g(\widetilde{H}_k)]])v),$$

an identity which allows us to conclude our proof easily. □

Proof of Lemma 5.10. If K is $\widetilde{H}_k$-compact, for all $u \in \mathrm{Dom}(\widetilde{H}_k)$ we have

$$\lim_{t\to\pm\infty} K(\widetilde{H}_k + \mathrm{i})^{-1}\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} P_{\mathrm{ac}}(\widetilde{H}_k)(\widetilde{H}_k + \mathrm{i})u = 0,$$

by the Riemann-Lebesgue lemma. Since $\mathrm{Dom}(\widetilde{H}_k)$ is dense we may conclude that

$$\mathrm{s}-\lim_{t\to\pm\infty} K\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} P_{\mathrm{ac}}(\widetilde{H}_k) = 0.$$

We note that for all $r, s > 0$, $\tilde{1}_k^{(r)} - \tilde{1}_k^{(s)}$ is $\widetilde{H}_k$-compact by Hypothesis (H2) (vii). Hypothesis (H1) (ii) and the inequalities (106) imply

$$0 \le \tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)} \le \tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2} \le \tilde{1}_k^{(r)} - \tilde{1}_k^{(r+1)},$$

and consequently $\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)}$ and $\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}$ are $\widetilde{H}_k$-compact. Thus, the operators $\widetilde{\chi}_k^{(r)2} P_{\mathrm{ac}}(\widetilde{H}_k) = M_k^{(r)*} M_k^{(r)} P_{\mathrm{ac}}(\widetilde{H}_k)$, $\widetilde{\chi}_k^{(r)} P_{\mathrm{ac}}(\widetilde{H}_k)$, $\tilde{1}_k^{(r)} P_{\mathrm{ac}}(\widetilde{H}_k)$, and $\tilde{1}_k P_{\mathrm{ac}}(\widetilde{H}_k)$ are asymptotically $\widetilde{H}_k$-equivalent and it suffices for us to consider the strong limits $\Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; \widetilde{\chi}_k P_{\mathrm{ac}}(\widetilde{H}_k))$. Furthermore, Hypothesis (H3) ensures that the spectrum of $\widetilde{H}_k$ is purely absolutely continuous on $\mathbb{R} \setminus \Sigma_k$. The Lebesgue measure of Σ_k being zero thus allows us to restrict to $\Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; \widetilde{\chi}_k g(\widetilde{H}_k)^2)$ where $g \in C_0^\infty(\mathbb{R} \setminus \Sigma_k)$ and $\widetilde{H}_k$ satisfy a strict Mourre estimate on $\Delta = \mathrm{supp}\, g$. A simple variation of Corollary 5.5 shows that $[\widetilde{\chi}_k, g(\widetilde{H}_k)]$ is compact. It thus suffices to consider the case of $\Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; g(\widetilde{H}_k)\widetilde{\chi}_k g(\widetilde{H}_k))$. We may now write, as a quadratic form,

$$[\widetilde{H}_k, g(\widetilde{H}_k)\widetilde{\chi}_k g(\widetilde{H}_k)] = g(\widetilde{H}_k)[\widetilde{H}_k, \widetilde{\chi}_k]g(\widetilde{H}_k) = C_k^* \widetilde{\Xi}_{k,g} C_k,$$

with $C_k = (\widetilde{A}_k^2 + 1)^{-1}$. The operator $\widetilde{\Xi}_{k,g}$ is bounded by Lemma 5.13. The existence of the strong limit $\Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; g(\widetilde{H}_k)\widetilde{\chi}_k g(\widetilde{H}_k))$ now follows from Corollary 4.26 and from Proposition 5.8.

Having established the existence of $\widetilde{P}_k^{\pm} = \Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; \tilde{1}_k P_{\mathrm{ac}}(\widetilde{H}_k))$, it follows from the general remarks in Section 5.4.2 that

$$\Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; \tilde{1}_k P_{\mathrm{ac}}(\widetilde{H}_k)) = \Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; P_{\mathrm{ac}}(\widetilde{H}_k)\tilde{1}_k P_{\mathrm{ac}}(\widetilde{H}_k)),$$

which implies that $\widetilde{P}_k^{\pm}$ is self-adjoint and that

$$\Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; \tilde{1}_k P_{\mathrm{ac}}(\widetilde{H}_k))^2 = \Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; \tilde{1}_k P_{\mathrm{ac}}(\widetilde{H}_k)).$$

This confirms that $\widetilde{P}_k^{\pm}$ is an orthogonal projection.

Finally, we note that $u \in \operatorname{Ran} \widetilde{P}_k^{\pm}$ if and only if, for all $r > 0$,

$$0 = \|u - \widetilde{P}_k^{\pm} u\| = \lim_{t \to \pm\infty} \|\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u - \tilde{1}_k^{(r)} \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u\| = \lim_{t \to \pm\infty} \|(I - \tilde{1}_k^{(r)}) \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} u\|.$$

The range of the projection $\widetilde{P}_k^{\mp}$ is thus $\widetilde{\mathscr{H}}_k^{\mathrm{in/out}}$. □

Proof of Proposition 5.11. We use the same approach as in the previous proof. We remark first that if $0 \le r \le s$, Hypothesis (H1) (vi) implies that

$$J_k^{(r)} - J_k^{(s)} = J_k^{(r)} (\tilde{1}_k^{(r)} - \tilde{1}_k^{(s)}),$$

and Hypothesis (H2) (vii) allows us to conclude that $J_k^{(r)} - J_k^{(s)}$ is $\widetilde{H}_k$-compact. $J_k^{(r)} P_{\mathrm{ac}}(\widetilde{H}_k)$ and $J_k^{(s)} P_{\mathrm{ac}}(\widetilde{H}_k)$ are thus asymptotically $\widetilde{H}_k$-equivalent, which shows that if the partial Møller operators exist, they are independent of choice of $r > 0$.

We note again that for all $r \ge 0$

$$(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)}) \tilde{1}_k^{(r)} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)}), \tag{124}$$

while Hypothesis (H1) (iv) implies

$$\tilde{1}_k^{(r)} \tilde{1}_k^{(r+1)} = \tilde{1}_k^{(r+1)}. \tag{125}$$

and identity (107) implies

$$\widetilde{\chi}_k^{(r)} \tilde{1}_k^{(r+1)} = \tilde{1}_k^{(r+1)}. \tag{126}$$

The relations (124),(125) and (126) allow us to conclude that

$$J_k^{(r)} - M_k^{(r)} = J_k^{(r)} (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)}) = J_k^{(r)} (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)}) (\tilde{1}_k^{(r)} - \tilde{1}_k^{(r+1)}),$$

is $\widetilde{H}_k$-compact by Hypothesis (H2) (vii). $J_k^{(r)}$ and $M_k^{(r)}$ are thus asymptotically $\widetilde{H}_k$-equivalent. To prove the existence of the partial Møller operators it is thus sufficient to consider the limits $\Gamma^{\pm}(H, \widetilde{H}_k; M_k P_{\mathrm{ac}}(\widetilde{H}_k))$. As in the proof of Lemma 5.10, we may restrict ourselves to $\Gamma^{\pm}(H, \widetilde{H}_k; M_k g(\widetilde{H}_k)^2)$ with $g \in C_0^\infty(\mathbb{R} \setminus S_k)$ where $S_k = \Sigma_k \cup \mathrm{Sp}_{\mathrm{pp}}(H)$ is discrete by Corollary 5.3 and H and $\widetilde{H}_k$ both satisfy a strict Mourre estimate on $\Delta = \operatorname{supp} g$. By invoking Corollary 5.5 it suffices for us to consider $\Gamma^{\pm}(H, \widetilde{H}_k; g(H) M_k g(\widetilde{H}_k))$. As a quadratic form we have

$$H g(H) M_k g(\widetilde{H}_k) - g(H) M_k g(\widetilde{H}_k) \widetilde{H}_k = C^* \, \Xi_{k,g} C_k,$$

with $C = (A^2 + 1)$, $C_k = (\widetilde{A}_k^2 + 1)$ and $\Xi_{k,g}$ bounded by Lemma 5.13. Invoking Theorem 5.2, we obtain the existence of $\Gamma^{\pm}(H, \widetilde{H}_k; g(H) M_k g(\widetilde{H}_k))$ and of $\Gamma^{\pm}(\widetilde{H}_k, H; g(\widetilde{H}_k) M_k^* g(H))$ as in the proof of Lemma 5.10. It follows that $\Omega_k^{\pm} = \Gamma^{\pm}(H, \widetilde{H}_k; M_k P_{\rm ac}(\widetilde{H}_k))$ and $\Omega_k^{\pm *} = \Gamma^{\pm}(\widetilde{H}_k, H; M_k^* P_{\rm ac}(H))$ exist. Hypothesis (H1) (iii) and Lemma 5.10 imply

$$\Omega_k^{\pm *}\Omega_l^{\pm} = \Gamma^{\pm}(\widetilde{H}_k, \widetilde{H}_k; M_k^* M_l P_{\rm ac}(H)) = \delta_{kl}\widetilde{P}_k^{\pm},$$

and thus $\operatorname{Ran}\Omega_k^{\pm *} = \widetilde{\mathscr{H}}_k^{\rm in/out}$. The inequality (118) and Hypothesis (H2) (vi) show that $I - \sum_{k=1}^{M} M_k M_k^*$ is H-compact, from which we get that

$$\begin{aligned}\sum_{k=1}^{M}\Omega_k^{\pm}\Omega_k^{\pm *} &= \sum_{k=1}^{M}\Gamma^{\pm}(H, H; M_k M_k^* P_{\rm ac}(H))\\ &= \Gamma^{\pm}(H, H; P_{\rm ac}(H)) = P_{\rm ac}(H).\end{aligned}$$

□

Proof of Corollary 5.12. Hypothesis (H1) (iii) (v) implies that, for $0 \le r \le s$,

$$1_k^{(r)} - 1_k^{(s)} = 1_k^{(r)}(1_k^{(r)} - 1_k^{(s)}) = 1_k^{(r)}(1_0^{(s)} - 1_0^{(r)}).$$

Hypothesis (H2) (vi) allows us to conclude that $1_k^{(r)} - 1_k^{(s)}$ is H-compact. $1_k^{(r)} P_{\rm ac}(H)$ and $1_k^{(s)} P_{\rm ac}(H)$ are thus asymptotically H-equivalent. Hypothesis (H1) (ii) (vi) implies

$$0 \le 1_k - M_k M_k^* = J_k(\tilde{1}_k - \tilde{\chi}_k^2)J_k^* \le J_k(\tilde{1}_k - \tilde{1}_k^{(2)})J_k^* = 1_k^{(1)} - 1_k^{(2)},$$

$1_k P_{\rm ac}(H)$ and $M_k M_k^* P_{\rm ac}(H)$ are thus asymptotically H-equivalent. We thus have

$$\begin{aligned}\Omega^{\pm}\widetilde{P}_k^{\pm}\Omega^{\pm *} = \Omega_k^{\pm}\Omega_k^{\pm *} &= \Gamma^{\pm}(H, H; M_k M_k^* P_{\rm ac}(H))\\ &= \Gamma^{\pm}(H, H; 1_k P_{\rm ac}(H))\\ &= \Gamma^{\pm}(H, H; 1_k^{(r)} P_{\rm ac}(H))\\ &= P_k^{\pm},\end{aligned}$$

for all $r \ge 0$. Since

$$P_k^{\pm *} = (\Omega_k^{\pm}\Omega_k^{\pm *})^* = \Omega_k^{\pm}\Omega_k^{\pm *} = P_k^{\pm},$$

and

$$P_k^{\pm}P_l^{\pm} = (\Omega_k^{\pm}\Omega_k^{\pm *})(\Omega_l^{\pm}\Omega_l^{\pm *}) = \Omega_k^{\pm}(\Omega_k^{\pm *}\Omega_l^{\pm})\Omega_l^{\pm *} = \delta_{kl}\Omega_k^{\pm}\widetilde{P}_k^{\pm}\Omega_k^{\pm *} = \delta_{kl}P_k^{\pm},$$

$P_k^{\pm}$ are the disjoint orthogonal projections. Furthermore

$$\sum_{k=1}^{M} P_k^{\pm} = \sum_{k=1}^{M}\Omega_k^{\pm}\Omega_k^{\pm *} = \Omega^{\pm}\Omega^{\pm *} = P_{\rm ac}(H).$$

Finally, $u \in \operatorname{Ran} P_k^{\pm}$ if and only if

$$0 = \|u - P_k^{\pm}u\| = \lim_{t\to\pm\infty}\|e^{-itH}u - 1_k^{(r)}e^{-itH}u\|,$$

for all $r \ge 0$. □

5.5 Non-equilibrium steady states (NESS)

We set $\mathcal{O}_k = \mathrm{CAR}(\widetilde{\mathcal{H}}_k)$ and we denote by τ_k^t the group of Bogoliubov automorphisms on $\mathcal{O}_k$ generated by $\widetilde{H}_k$. The following result is a slightly adapted version of Theorem 3.2 of [AJPP2]. This is the fundamental result which ensures the existence of a rich enough family of nonequilibrium steady states.

Proposition 5.14 *We suppose Hypotheses (H1) and (H2) hold. For all $k \in \{1,\dots,M\}$ let $\widetilde{T}_k \in \mathcal{B}(\widetilde{\mathcal{H}}_k)$ be the generator of a gauge invariant quasi-free state which is also τ_k-invariant on $\mathcal{O}_k$. Then, for all $r \geq 0$,*

$$T = \sum_{k=1}^{M} J_k^{(r)} \widetilde{T}_k J_k^{(r)*},$$

generates a gauge invariant quasi-free state ω_T on $\mathcal{O}$. If Hypothesis (H3) also holds, the NESS

$$\omega_T^+ = \mathrm{w}^*-\lim_{t\to\infty} \frac{1}{t}\int_0^t \omega_T \circ \tau^s \,\mathrm{d}s, \tag{127}$$

exists. Furthermore, the following hold.

(i) The restriction $\omega_T^+|_{\mathrm{CAR}(\mathcal{H}_{\mathrm{ac}})}$ is the gauge invariant quasi-free state generated by

$$T^+ = \sum_{k=1}^{M} \Omega_k^- \widetilde{T}_k \Omega_k^{-*}.$$

In particular, this state does not depend on $r \geq 0$.

(ii) For any gauge invariant and ω_T-normal state η on $\mathcal{O}$ and for all $A \in \mathrm{CAR}(\mathcal{H}_{\mathrm{ac}})$,

$$\lim_{t\to\infty} \eta\circ\tau^t(A) = \omega_{T^+}(A).$$

(iii) For each trace-class operator c on $\mathcal{H}$,

$$\omega_T^+(\mathrm{d}\Gamma(c)) = \mathrm{tr}(T^+c) + \sum_{\varepsilon\in \mathrm{Sp}_{\mathrm{pp}}(H)} \mathrm{tr}(P_\varepsilon T P_\varepsilon c), \tag{128}$$

where P_ε denotes the orthogonal projection onto the eigenspace of H associated to the eigenvalue ε.

Proof. By hypothesis we have $0 \leq \widetilde{T}_k \leq I$ for all $k \in \{1,\dots,M\}$. By invoking Hypothesis (H1) we get that

$$\begin{aligned}(u, Tu) &= \sum_{k=1}^{M} (J_k^{(r)*}u, \widetilde{T}_k J_k^{(r)*}u) \leq \sum_{k=1}^{M} (J_k^{(r)*}u, J_k^{(r)*}u)\\ &= \sum_{k=1}^{M} (u, 1_k^{(r)*}u) = (u, (I - 1_0^{(r)})u) \leq (u,u),\end{aligned}$$

and thus $0 \leq T \leq I$ which shows that T is the generator of a gauge invariant quasi-free state on $\mathscr{O}$.

The rest of the proposition is proven like Theorem 3.2 of [AJPP2], by remarking that

$$\begin{aligned}\lim_{t\to\infty}(\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)g, T\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)f) &= \sum_{k=1}^{M}\lim_{t\to\infty}(\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}J_k^{(r)*}\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)g, \widetilde{T}_k\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}J_k^{(r)*}\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)f)\\ &= (g, T^+f).\end{aligned}$$

□

It is clear that the τ_k-invariance of $\omega_{\widetilde{T}_k}$, that is to say the fact that, for all $t \in \mathbb{R}$, $\mathrm{e}^{\mathrm{i}t\widetilde{H}_k}\widetilde{T}_k\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} = \widetilde{T}_k$ is crucial in the preceding proposition. We may choose for example $\widetilde{T}_k = f_k(\widetilde{H}_k)$ where $f_k : \mathrm{Sp}(\widetilde{H}_k) \to [0,1]$ is a measurable function. We therefore have, since $f(H)$ and P_k^- commute,

$$T^+ = \sum_{k=1}^{M}\Omega_k^- f_k(\widetilde{H}_k)\Omega_k^{-*} = \sum_{k=1}^{M} f_k(H)\Omega_k^-\Omega_k^{-*} = \oplus_{k=1}^{M}P_k^- f_k(H)P_k^-. \tag{129}$$

The particular case

$$f_k(\varepsilon) = \frac{1}{1+\mathrm{e}^{\beta_k(\varepsilon-\mu_k)}},$$

of course plays a crucial role in applications to statistical mechanics (recall Section 3.2.3).

The following result shows that we can, in an equivalent fashion, choose ω_T as a “superposition” of τ-invariant states.

Theorem 5.15 *We suppose that Hypotheses (H1) and (H2) hold. For all $k \in \{1,\dots,M\}$ let $T_k \in \mathscr{B}(\mathscr{H})$ be the generator of a gauge invariant, quasi-free state which is also τ-invariant on $\mathscr{O}$. Then, for all $r \geq 0$,*

$$T = \sum_{k=1}^{M} 1_k^{(r)}T_k 1_k^{(r)},$$

generates a gauge invariant quasi-free state on $\mathscr{O}$. If Hypothesis (H3) also holds, the NESS (127) exists and Assertions (i)-(iii) of Proposition 5.14 hold true with

$$T^+ = \sum_{k=1}^{M} P_k^- T_k P_k^- = \sum_{k=1}^{M}\Omega_k^-\widetilde{T}_k\Omega_k^{-*},$$

where $\widetilde{T}_k = \Omega_k^{-*}T_k\Omega_k^-$. In particular, if $T_k = f_k(H)$, we obtain the formula

$$T^+ = \sum_{k=1}^{M} P_k^- f_k(H)P_k^-,$$

which is identical to (129).

Proof. We argue in the same manner as in the proof of Proposition 5.14, by remarking that this time

$$\lim_{t\to\infty}(\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)g, T\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)f) =$$

$$\sum_{k=1}^{M}\lim_{t\to\infty}(\mathrm{e}^{-\mathrm{i}H}1_k^{(r)*}\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)g, T_k\mathrm{e}^{-\mathrm{i}tH}1_k^{(r)*}\mathrm{e}^{\mathrm{i}tH}P_{\mathrm{ac}}(H)f)$$

$$= (g, T^+ f).$$

□

6 The geometric Landauer-Büttiker formula

In this section we derive a Landauer-Büttiker formula for currents associated to a general class of conserved charges. As opposed to previous derivations of this formula [AJPP2, N] or of its linearized version [CJM], which exploit the stationary formalism of scattering theory we shall continue to use the time dependent framework.

6.1 Hypotheses

In the remaining parts of these notes, and unless otherwise stated, we shall assume that Hypotheses (H1), (H2), and (H3) of Section 5 hold. To establish the existence of current observable and to study their properties we must however make a few additional hypotheses.

(H4) There exists an integer $m > 2$ such that, for $k \in \{1, \dots, M\}$,

- (i) $(\widetilde{A}_k + \mathrm{i})^{-m} g(\widetilde{H}_k)$ is trace-class for all $g \in C_0^\infty(\mathbb{R} \setminus \Sigma_k)$.
- (ii) $\widetilde{H}_k \in \mathscr{B}^{m+2}_{\widetilde{A}_k}(\widetilde{\mathscr{H}}^1_k, \widetilde{\mathscr{H}}_k)$.
- (iii) $1_0^{(r)} g(H)$ is trace-class for all $g \in C_0^\infty(\mathbb{R})$ and $0 \le r \le 2$.

(H5) There exists an integer $\nu \ge 1$ such that, for $k \in \{1, \dots, M\}$,

- (i) $\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \in \mathscr{B}(\widetilde{\mathscr{H}}_k^{j/2}, \widetilde{\mathscr{H}}_k)$ for $j = 1, \dots, 4\nu$.
- (ii) $(I - \tilde{1}_k^{(r)})\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) = 0$ for $j = 1, \dots, 2\nu$.
- (iii) $\tilde{1}_k^{(r+1)}\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) = 0$ for $j = 1, \dots, 2\nu$.
- (iv) $(\widetilde{\chi}_k^{(r)} - \widetilde{\chi}_k^{(s)})(\widetilde{H}_k + \mathrm{i})^{-\nu}$ is trace-class for $r, s \ge 0$.

We insist on the fact that only Hypothesis (H4) (iii) concerns the sample $\mathfrak{S}$ through the Hamiltonian H. Moreover, this hypothesis, which quantifies the confinement of $\mathfrak{S}$ is very weak. All the other hypotheses concern only the extended reservoirs $\widetilde{\mathfrak{R}}_k$.

We begin by deducing several important consequences of these hypotheses which will be useful to us later on.

Lemma 6.1 *Under hypotheses (H1), (H2), and (H5) the operators*

$$(H-z)^{-\ell} M_k^{(r)} - M_k^{(r)} (\widetilde{H}_k - z)^{-\ell},$$

and

$$D_k^{(r)}(f) = f(H) M_k^{(r)} - M_k^{(r)} f(\widetilde{H}_k),$$

are trace-class for all $f \in C_0^\infty(\mathbb{R})$, $k \in \{1, \ldots, M\}$, $r \geq 1$, $z \in \mathrm{Res}(H) \cap \mathrm{Res}(\widetilde{H}_k)$ *and* $\ell \geq \nu$.

The proof of this lemma being quite long and technical, we have chosen to defer it to Appendix A.

Lemma 6.2 *Under the hypotheses of Lemma 6.1 the operators*

$$\begin{array}{llll} [f(\widetilde{H}_k), \widetilde{\chi}_k^{(r)}], & [f(\widetilde{H}_k), \tilde{1}_k^{(r)}], & f(\widetilde{H}_k)(\widetilde{\chi}_k^{(r)} - \widetilde{\chi}_k^{(s)}) & f(\widetilde{H}_k)(\tilde{1}_k^{(r)} - \tilde{1}_k^{(s)}) \\ [f(H), \chi_k^{(r)}], & [f(H), 1_k^{(r)}], & f(H)(\chi_k^{(r)} - \chi_k^{(s)}) & f(H)(1_k^{(r)} - 1_k^{(s)}), \end{array}$$

are trace-class for all $f \in C_0^\infty(\mathbb{R})$, $k \in \{1, \ldots, M\}$ *and* $r, s \geq 1$.

Proof. Hypothesis (H5) (iv) implies that for $r, s \geq 0$

$$f(\widetilde{H}_k)(\widetilde{\chi}_k^{(r)} - \widetilde{\chi}_k^{(s)}) = f(\widetilde{H}_k)(\widetilde{H}_k + \mathrm{i})^{\nu} (\widetilde{H}_k + \mathrm{i})^{-\nu} (\widetilde{\chi}_k^{(r)} - \widetilde{\chi}_k^{(s)}),$$

is trace-class. We set $D \equiv D_k^{(r)}(f)$ and remark that Lemma 6.1 implies that, for $r \geq 1$,

$$[f(\widetilde{H}_k), \widetilde{\chi}_k^{(r)2}] = f(\widetilde{H}_k) M_k^{(r)*} M_k^{(r)} - M_k^{(r)*} M_k^{(r)} f(\widetilde{H}_k) = M_k^{(r)*} D - D^* M_k^{(r)},$$

is trace-class. Hypothesis (H1) (iv) and Identity (107) imply

$$(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}) \widetilde{\chi}_k^{(r+1)} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}) \tilde{1}_k^{(r+1)} \widetilde{\chi}_k^{(r+1)} = (\tilde{1}_k^{(r+1)} - \tilde{1}_k^{(r+1)}) \widetilde{\chi}_k^{(r+1)} = 0,$$

$$(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}) \widetilde{\chi}_k^{(r-1)} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}) \tilde{1}_k^{(r)} \widetilde{\chi}_k^{(r-1)} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}) \tilde{1}_k^{(r)} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}),$$

from which we conclude that

$$\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2})(\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)}) = (\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)})(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}). \tag{130}$$

In the same way, one shows that

$$\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)} = (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)})(\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)}) = (\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)})(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)}). \tag{131}$$

From (130) we get that

$$
\begin{aligned}
[f(\widetilde{H}_k), \tilde{1}_k^{(r)}] = [f(\widetilde{H}_k), \widetilde{\chi}_k^{(r)2}] &+ f(\widetilde{H}_k)(\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)})(\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2}) \\
&- (\tilde{1}_k^{(r)} - \widetilde{\chi}_k^{(r)2})(\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)}) f(\widetilde{H}_k),
\end{aligned}
$$

and Hypothesis (H5) (iv) allows us to conclude that $[f(\widetilde{H}_k), \tilde{1}_k^{(r)}]$ is trace-class. In an analogous manner we deduce from (131) that $[f(\widetilde{H}_k), \widetilde{\chi}_k^{(r)}]$ is trace-class. Since

$$
\begin{aligned}
[f(H), \chi_k^{(r)}] &= f(H) M_k^{(r)} J_k^{(r)*} - J_k^{(r)} M_k^{(r)*} f(H) \\
&= M_k^{(r)} f(\widetilde{H}_k) J_k^{(r)*} + D J_k^{(r)*} - J_k^{(r)} f(\widetilde{H}_k) M_k^{(r)*} - J_k^{(r)} D^* \\
&= -J_k^{(r)} [f(\widetilde{H}_k), \widetilde{\chi}_k^{(r)}] J_k^{(r)*} + D J_k^{(r)*} - J_k^{(r)} D^*,
\end{aligned}
$$

we may also conclude that $[f(H), \chi_k^{(r)}]$ is trace-class. The identity

$$
\begin{aligned}
f(H)(\chi_k^{(r)} - \chi_k^{(s)}) &= f(H)(M_k^{(r)} J_k^{(r)*} - M_k^{(s)} J_k^{(s)*}) \\
&= (f(H) M_k^{(r)} - M_k^{(r)} f(\widetilde{H}_k)) J_k^{(r)*} \\
&\quad - (f(H) M_k^{(s)} - M_k^{(s)} f(\widetilde{H}_k)) J_k^{(s)*} \\
&\quad + J_k^{(s)} [f(\widetilde{H}_k), \widetilde{\chi}_k^{(s)}] J_k^{(s)*} - J_k^{(r)} [f(\widetilde{H}_k), \widetilde{\chi}_k^{(r)}] J_k^{(r)*} \\
&\quad + J_k^{(r)} f(\widetilde{H}_k)(\widetilde{\chi}_k^{(r)} - \widetilde{\chi}_k^{(s)}) J_k^{(r)*},
\end{aligned}
$$

implies that $f(H)(\chi_k^{(r)} - \chi_k^{(s)})$ is trace-class for $r, s \geq 1$. The identity

$$
1_k^{(r)} - \chi_k^{(r)} = (1_k^{(r)} - \chi_k^{(r)})(\chi_k^{(r-1)} - \chi_k^{(r+1)}) = (\chi_k^{(r-1)} - \chi_k^{(r+1)})(1_k^{(r)} - \chi_k^{(r)}), \tag{132}
$$

(a version of (131) without tilde) allows us to show that $[f(H), 1_k^{(r)}]$ is trace-class. Finally, one deduces from Identities (131), (132) and the previous results that $f(\widetilde{H}_k)(\tilde{1}_k^{(r)} - \tilde{1}_k^{(s)})$ and $f(H)(1_k^{(r)} - 1_k^{(s)})$ are trace class. □

Lemma 6.3 *If Hypotheses (H1)–(H5) are satisfied, then $f(H)\chi_k^{(r)} g(A_k)$ and $f(H) 1_k^{(r)} g(A_k)$ are trace-class for all $r \geq 1$, $f \in C_0^\infty(\mathbb{R} \setminus \Sigma_H)$ and $g \in C_0^\infty(\mathbb{R})$.*

Proof. Since $A_k = J_k \widetilde{A}_k J_k^*$, we have

$$
(A_k - z)^{-1} = J_k(\widetilde{A}_k - z)^{-1} J_k^* - z^{-1}(I - 1_k),
$$

and the Helffer-Sjöstrand formula yields

$$
g(A_k) = J_k g(\widetilde{A}_k) J_k^* - g(0)(I - 1_k), \tag{133}
$$

for all $g \in C_0^\infty(\mathbb{R})$. We thus have

$$\begin{aligned} f(H)\chi_k^{(r)} g(A_k) &= f(H) M_k^{(r)} g(\widetilde{A}_k) J_k^* \\ &= (f(H)M_k^{(r)} - M_k^{(r)} f(\widetilde{H}_k)) g(\widetilde{A}_k) J_k^* \\ &+ M_k^{(r)} f(\widetilde{H}_k)(\widetilde{A}_k + \mathrm{i})^{-m}(\widetilde{A}_k + \mathrm{i})^m g(\widetilde{A}_k) J_k^*, \end{aligned}$$

and Hypotheses (H4) (i) and Lemma 6.1 imply the first assertion. Writing

$$f(H)1_k^{(r)} g(A_k) = f(H)\chi_k^{(r)} g(A_k) + f(H)(1_k^{(r)} - \chi_k^{(r)}) g(A_k),$$

the second assertion is a direct consequence of the first one, Identity (131) and Lemma 6.2. □

We note for later reference that Identity (111) implies

$$J_k^{(r)}(\widetilde{A}_k - z)^{-j} J_k^{(r)*} = M_k^{(r)}(\widetilde{A}_k - z)^{-j} M_k^{(r)*} + (-z)^{-j}(1_k^{(r)} - M_k^{(r)} M_k^{(r)*}), \tag{134}$$

for $z \in \mathbb{C} \setminus \mathbb{R}$ and $j \in \mathbb{N}$, and hence

$$J_k^{(r)} g(\widetilde{A}_k) J_k^{(r)*} = M_k^{(r)} g(\widetilde{A}_k) M_k^{(r)*} - g(0)(1_k^{(r)} - M_k^{(r)} M_k^{(r)*}).$$

Together with Eq. (133), we thus obtain

$$g(A_k) = M_k^{(r)} g(\widetilde{A}_k) M_k^{(r)*} - g(0)(I - M_k^{(r)} M_k^{(r)*}). \tag{135}$$

6.2 A simple model (continued)

We come back to the simple example of Section 5.2. As already remarked there, Hypotheses (H4) (ii) holds for any integer m. For any $\nu \geq 1$, the verification of Hypotheses (H5) (ii)–(iii) reduces to straightforward calculations while (H5) (i) follows from the easily established fact that

$$\mathrm{ad}^n_{\widetilde{H}_\mp}(\widetilde{\chi}_\mp^{(r)}) = \sum_{j=0}^n c_{nj}(x)\partial_x^j,$$

with $c_{nj} \in C_0^\infty(\mathbb{R})$. To check the remaining Hypotheses (H4) (i)+(iii) and (H5) (iv) we need some trace-class estimates.

For any $r > 0$ there exists a compact subset $K \subset \mathfrak{M}$ such that $1_0^{(r)} g(H) = 1_0^{(r)} 1_K (H+1)^{-s}(H+1)^s g(H)$ holds for any $s > 0$ (1_K denotes the operator of multiplication by the characteristic function of K). Reciprocally, for any compact subset $K \subset \mathfrak{M}$ and $s \geq 1$ one has $1_K(H+1)^{-s} = 1_K 1_0^{(r)}(H+1)^{-1}(H+1)^{-(s-1)}$ for large enough $r > 0$. Thus, to prove Property (H4) (iii) it suffices to show that for sufficiently large $s > 0$ and any compact subset $K \subset \mathfrak{M}$ the operator $1_K(H+1)^{-s}$ is trace-class. Moreover, we already know, from Hypothesis (H2) (vi), that this operator is compact. Set $C = (H+1)^{-s} 1_K$ and denote by $\{\mu_j\}$ the decreasing sequence of repeated eigenvalues of $C^* C = 1_K (H+1)^{-2s} 1_K \geq 0$. We have to show that

$$\|C\|_1 = \mathrm{tr}|C| = \sum_j \mu_j^{1/2} < \infty. \tag{136}$$

Since $\mathrm{Sp}(AB)\setminus\{0\} = \mathrm{Sp}(BA)\setminus\{0\}$ holds for any bounded operators A and B, the sequence $\{\mu_j\}$ coincide with the sequence of non-zero eigenvalues of $\widetilde{C} = 1_K(H+1)^{-2s}$. By Proposition 1 and Theorem 3 in [Sk], we have

$$\mu_j = \mathcal{O}(j^{-2s}),$$

as $j\to\infty$ so that (136) holds provided $s>1$. We can use the same argument to show that Hypothesis (H5) (iv) holds provided $\nu>1$.

The case of Hypothesis (H4) (i) is more delicate. We first claim that we can replace $\widetilde{A}_\mp$ with the generator $A_0 = \frac{1}{2\mathrm{i}}(x\partial_x + \partial_x x)$ of the dilation group $(U_0^t f)(x,\varphi) = \mathrm{e}^{t/2} f(\mathrm{e}^t x,\varphi)$. Indeed, with $\chi\in C_0^\infty(\mathbb{R})$ such that $0\le\chi(x)\le 1$ for all $x\in\mathbb{R}$ and $\chi(x)=1$ for $|x|\le 20$ we can write

$$(\widetilde{A}_\mp+\mathrm{i})^{-m} g(\widetilde{H}_\mp) = (\widetilde{A}_\mp+\mathrm{i})^{-m}\chi(x) g(\widetilde{H}_\mp) + (\widetilde{A}_\mp+\mathrm{i})^{-m}(I-\chi(x))(A_0+\mathrm{i})^m(A_0+\mathrm{i})^{-m} g(\widetilde{H}_\mp).$$

The first term on the right hand side of this identity is trace class by the argument previously used to prove Hypothesis (H5) (iv). To deal with the second term, we invoke Lemma 4.7 and use the fact that $v(x)=x$ on the support of $1-\chi$ to write

$$\begin{aligned}(\widetilde{A}_\mp+\mathrm{i})^{-m}(I-\chi(x))(A_0+\mathrm{i})^m &= (\widetilde{A}_\mp+\mathrm{i})^{-m}(I-\chi(x))(A_\mp+\mathrm{i})^m\\ &= I-\chi(x) + [(\widetilde{A}_\mp+\mathrm{i})^{-m},(I-\chi(x))](A_\mp+\mathrm{i})^m\\ &= I-\chi(x) - \sum_{j=1}^m \binom{m}{j}\mathrm{i}^j(\widetilde{A}_\mp+\mathrm{i})^{-j}\mathrm{ad}^j_{\widetilde{A}_\mp}(\chi).\end{aligned}$$

Since $\mathrm{ad}^j_{\widetilde{A}_\mp}(\chi) = (v(x)\partial_x)^j\chi\in C_0^\infty(\mathbb{R})$, we conclude that $(\widetilde{A}_\mp+\mathrm{i})^{-m}(I-\chi(x))(A_0+\mathrm{i})^m$ is bounded. Thus, as claimed, it is sufficient to show that $(A_0+\mathrm{i})^{-m} g(\widetilde{H}_\mp)$ is trace class.

We shall derive a more convenient representation of this operator using the following unitary maps:

1. The Fourier transform $\mathscr{F}:\widetilde{\mathscr{H}}_\mp = L^2(\mathbb{R}\times\gamma_\mp, \mathrm{d}x\,R\mathrm{d}\varphi)\to L^2(\mathbb{R},\mathrm{d}p)\otimes\ell^2(\mathbb{Z})$,

$$(\mathscr{F}f)(p,k) = \frac{R^{1/2}}{2\pi}\int_{\mathbb{R}}\mathrm{d}x\int_0^{2\pi}\mathrm{d}\varphi\, f(x,\varphi)\mathrm{e}^{-\mathrm{i}(px+k\varphi)},$$

   maps the Hamiltonian $\widetilde{H}_\mp$ to the multiplication operator

$$(\mathscr{F}\widetilde{H}_\mp f)(p,k) = (p^2+\lambda_k^2)(\mathscr{F}f)(p,k),$$

   and the dilation group U_0^t to its inverse, $(\mathscr{F}U_0^t f)(p,k) = \mathrm{e}^{-t/2}(\mathscr{F}f)(\mathrm{e}^{-t}p,k)$.

2. The map $\mathscr{P}: L^2(\mathbb{R},\mathrm{d}p)\otimes\ell^2(\mathbb{Z})\to L^2(\mathbb{R}_+,\mathrm{d}p)\otimes\mathbb{C}^2\otimes\ell^2(\mathbb{Z})$ defined by

$$(\mathscr{P}f)(p,k) = \frac{1}{\sqrt{2}}\begin{pmatrix} f(-p,k)-f(p,k)\\ f(-p,k)+f(p,k)\end{pmatrix} = \begin{pmatrix}(\mathscr{P}f)_-(p,k)\\ (\mathscr{P}f)_+(p,k)\end{pmatrix},$$

   decomposes f into its odd/even parts w.r.t. the p-variable. It clearly commutes with the actions of $\widetilde{H}_\mp$ and U_0^t.

3. The map $\mathscr{V} : L^2(\mathbb{R}_+, \mathrm{d}p) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z}) \to L^2(\mathbb{R}, \mathrm{d}s) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$ defined by
$$(\mathscr{V} f)(s,k) = \mathrm{e}^{s/2} f(\mathrm{e}^s, k),$$
implements the change of variable $s = \log p$.
4. The Fourier transform in the s-variable $\mathscr{S} : L^2(\mathbb{R}, \mathrm{d}s) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z}) \to L^2(\mathbb{R}, \mathrm{d}a) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$,
$$(\mathscr{S} f)(a,k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}as} f(s,k) \mathrm{d}s.$$
5. The Mellin transform $\mathscr{M} = \mathscr{S}\mathscr{V} : L^2(\mathbb{R}_+, \mathrm{d}p) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z}) \to L^2(\mathbb{R}, \mathrm{d}a) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$,
$$(\mathscr{M} f)(a,k) = \frac{1}{\sqrt{2\pi}} \int_0^\infty p^{\mathrm{i}a-1/2} f(p,k) \mathrm{d}p,$$
satisfies $(\mathscr{M}\mathscr{P}\mathscr{F} U_0^t f)(a,k) = \mathrm{e}^{\mathrm{i}ta}(\mathscr{M}\mathscr{P}\mathscr{F} f)(a,k)$. Thus, $\mathscr{M}\mathscr{P}\mathscr{F}$ maps the operator A_0 to a multiplication operator $(\mathscr{M}\mathscr{P}\mathscr{F} A_0 f)(a,k) = a(\mathscr{M}\mathscr{P}\mathscr{F} f)(a,k)$.

It follows that $(A_0 + \mathrm{i})^{-m} g(\widetilde{H}_\mp) = \mathscr{F}^* \mathscr{P}^* \mathscr{M}^* C \mathscr{V} \mathscr{P} \mathscr{F}$ where C is the operator acting on $L^2(\mathbb{R}) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$ as
$$(Cf)_\pm(a,k) = F(a)(\mathscr{S} G_k f_\pm(\cdot, k))(a),$$
where $F(a) = (a+\mathrm{i})^{-m}$ and G_k is the operator of multiplication by the function $G_k(s) = g(\mathrm{e}^{2s} + \lambda_k^2)$. Writing our Hilbert space as a direct sum
$$L^2(\mathbb{R}) \otimes \mathbb{C}^2 \otimes \ell^2(\mathbb{Z}) = \bigoplus_{\langle k,\sigma\rangle \in \mathbb{Z}\times\{\pm\}} L^2(\mathbb{R}),$$
and denoting by $C_{k\pm}$ the operator defined on $L^2(\mathbb{R})$ by $(C_{k\pm} f)(a) = F(a)(\mathscr{S} G_k f)(a)$ we get
$$C = \bigoplus_{\langle k,\sigma\rangle \in \mathbb{Z}\times\{\pm\}} C_{k\sigma}.$$
Let $\delta = \operatorname{dist}(\operatorname{supp}(g), \Sigma_\pm) > 0$ and $\rho = \sup \operatorname{supp}(g)$. For $s \in \operatorname{supp}(G_k)$ one has
$$\inf_{j\in\mathbb{Z}} |\mathrm{e}^{2s} + \lambda_k^2 - \lambda_j^2| \ge \delta, \qquad \mathrm{e}^{2s} + \lambda_k^2 \le \rho.$$
It follows that $G_k \in C_0^\infty(\mathbb{R})$ with
$$\begin{cases} G_k = 0 & \text{if } |k| > R\rho^{1/2}; \\ \operatorname{supp}(G_k) \subset [\log(\delta)/2, \log(\rho)/2] & \text{otherwise.} \end{cases}$$
Thus, it suffices to show that $C_{k\pm}$ is trace class for any $\langle k,\sigma\rangle \in \mathbb{Z}\times\{\pm\}$.

The (quasi-)Banach space $\ell^p(\mathbb{Z}, L^2([0,1]))$ is the space of measurable functions $f : \mathbb{R} \to \mathbb{C}$ such that
$$\|f\|_{2,p} = \left(\sum_{j\in\mathbb{Z}} \left(\int_0^1 |f(j+s)|^2 \mathrm{d}s \right)^{p/2} \right)^{1/p} < \infty.$$

One easily checks that $\|F\|_{2,p} < \infty$ for $p > m^{-1}$ and $\|G_k\|_{2,p} < \infty$ for any $p > 0$. It follows from Paragraph 5.7 in [BKS] (see also Theorem 4.5 in [S]) that the singular values of $C_{k\pm}$ satisfy

$$\kappa_j(C_{k\pm}) = \mathcal{O}(j^{-1/p}),$$

as $j \to \infty$ for any $p > m^{-1}$. In particular, $C_{k\pm}$ is trace-class for $m > 1$.

The arguments presented in this section can easily be adapted to the various extensions discussed at the end of Section 5.2. We note however that Hypothesis (H4) (i) fails for super-reservoirs of the type $\widetilde{\mathfrak{R}}_j =]1, \infty[\times \gamma_j$ equipped with a metric $g_{\widetilde{\mathfrak{R}}_j} = \mathrm{d}x^2 + r(x)^2 g_{\gamma_j}$, such that $r(x) \to \infty$ as $x \to \infty$. In fact, it follows from Hypotheses (H1)–(H5) that the Hamiltonian H has locally finite spectral multiplicity (see Proposition B.3). In physical terms, our hypotheses only allow for a finite number of open scattering channels at any given finite energy E.

6.3 Charges and conserved currents

6.3.1 Charges

Definition 6.4 *A charge of the of one-particle system is an observable, described by the self-adjoint operator Q on $\mathcal{H}$, such that*

(i) $\mathrm{e}^{\mathrm{i}tH} Q \mathrm{e}^{-\mathrm{i}tH} = Q$ *for all* $t \in \mathbb{R}$.

(ii) For each $k \in \{1, \ldots, M\}$ *there exists a self-adjoint operator* $\widetilde{Q}_k$ *on* $\widetilde{\mathcal{H}}_k$ *such that*

$$\mathrm{e}^{\mathrm{i}t\widetilde{H}_k} \widetilde{Q}_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} = \widetilde{Q}_k,$$

for all $t \in \mathbb{R}$.

(iii) For each scattering state $u \in \mathcal{H}_\mathrm{s}$ *and for all* $r \geq 0$ *we have*

$$\lim_{t \to \pm\infty} \sum_{k=1}^{M} (M_k^{(r)*} \mathrm{e}^{-\mathrm{i}tH} u, \widetilde{Q}_k M_k^{(r)*} \mathrm{e}^{-\mathrm{i}tH} u) = (u, Qu).$$

Condition (i) expresses charge conservation in the system. Conditions (ii) and (iii) ensure that it is possible to determine the total charge of a scattering state by performing a measurement in the reservoirs (and waiting long enough). They reflect the fact that charge transport across the sample can be determined by measuring the charges in the reservoirs at two well separated times, as in the full counting scheme described in Section 3.4.8.

Since Condition (ii) implies

$$(M_k^{(r)*} \mathrm{e}^{-\mathrm{i}tH} u, \widetilde{Q}_k M_k^{(r)*} \mathrm{e}^{-\mathrm{i}tH} u) = (\mathrm{e}^{\mathrm{i}t\widetilde{H}_k} M_k^{(r)*} \mathrm{e}^{-\mathrm{i}tH} u, \widetilde{Q}_k \mathrm{e}^{\mathrm{i}t\widetilde{H}_k} M_k^{(r)*} \mathrm{e}^{-\mathrm{i}tH} u),$$

Condition (iii) is equivalent to

$$\sum_{k=1}^{M}(u_k^{\mathrm{in/out}},\widetilde{Q}_k u_k^{\mathrm{in/out}})=\sum_{k=1}^{M}(\Omega_k^{\mp *}u,\widetilde{Q}_k\Omega_k^{\mp *}u)=(u,Qu),$$

that is to say that $\mathcal{H}_{\mathrm{s}}=\mathcal{H}_{\mathrm{ac}}$ and

$$Q|_{\mathcal{H}_{\mathrm{ac}}}=\sum_{k=1}^{M}\Omega_k^{+}\widetilde{Q}_k\Omega_k^{+*}=\sum_{k=1}^{M}\Omega_k^{-}\widetilde{Q}_k\Omega_k^{-*}.$$

We have in particular

$$\Omega_k^{\pm *}Q\Omega_k^{\pm}=\widetilde{P}_k^{\pm}\widetilde{Q}_k\widetilde{P}_k^{\pm}, \tag{137}$$

and, by setting $\widetilde{Q}=\oplus_{k=1}^{M}\widetilde{Q}_k$,

$$Q|_{\mathcal{H}_{\mathrm{ac}}}=\Omega^{+}\widetilde{Q}\Omega^{+*}=\Omega^{-}\widetilde{Q}\Omega^{-*}. \tag{138}$$

We note that this condition implies

$$S\left(\widetilde{Q}\,|_{\widetilde{\mathcal{H}}^{\mathrm{in}}}\right)S^{*}=\widetilde{Q}\,|_{\widetilde{\mathcal{H}}^{\mathrm{out}}}, \tag{139}$$

which expresses the fact that the total charge of the reservoirs is conserved by the scattering process.

The two canonical examples of charge are the following.

1. The electric charge: by supposing that each fermion carries a unit charge, the observable of electric charge is simply $Q=I$. The corresponding observables in the reservoirs are $\widetilde{Q}_k=I$. Conditions (i) and (ii) are thus trivially satisfied. Condition (iii), or more precisely the equivalent condition (138) reduces to

$$P_{\mathrm{ac}}(H)=\Omega^{\pm}\Omega^{\pm *},$$

   that is to say to asymptotic completeness.

2. The energy: corresponds to $Q=H$ and $\widetilde{Q}_k=\widetilde{H}_k$. Conditions (i) and (ii) are again trivially satisfied, while (138) translates into

$$H_{\mathrm{ac}}=\Omega^{\pm}\left(\oplus_{k=1}^{M}\widetilde{H}_k\right)\Omega^{\pm *}.$$

6.3.2 Currents and regularized currents

Let Q be a charge of the one-particle system. The total charge in reservoir $\mathfrak{R}_k$ at a "distance" greater than r of the sample $\mathfrak{S}$ is described by the observable $\mathrm{d}\Gamma(1_k^{(r)}Q1_k^{(r)})$. The observable of the corresponding current is

$$\frac{\mathrm{d}}{\mathrm{d}t}\tau^{t}(\mathrm{d}\Gamma(1_k^{(r)}Q1_k^{(r)}))\bigg|_{t=0}=\mathrm{d}\Gamma(\mathrm{i}[H,1_k^{(r)}Q1_k^{(r)}]).$$

Our goal in this section is to give a meaning to the notion of steady current

$$\omega_T^+(\mathrm{d}\Gamma(\mathrm{i}[H, 1_k^{(r)} Q 1_k^{(r)}])), \tag{140}$$

expectation value of the current observable in the NESS which we constructed in Section 5. Several problems arise:

1. If the charge Q is an unbounded operator, the product $1_k^{(r)} Q 1_k^{(r)}$ does not make sense in general. This is the case, for example, for the energy current.

2. The commutator $[H, 1_k^{(r)} Q 1_k^{(r)}]$ is not well defined, even if Q is bounded.

3. To be able to use Assertion (iii) of Proposition 5.14 for the calculation of the expectation value of the current, the operator $[H, 1_k^{(r)} Q 1_k^{(r)}]$ must be trace-class

The appearance of these problems is not really a surprise. In fact, if the operator $\mathrm{d}\Gamma(1_k^{(r)} Q 1_k^{(r)})$ was a *bona fide* observable then its expectation

$$\omega_T^+ \circ \tau^t(\mathrm{d}\Gamma(1_k^{(r)} Q 1_k^{(r)})) = \mathrm{tr}(T^+ \mathrm{e}^{\mathrm{i}tH} 1_k^{(r)} Q 1_k^{(r)} \mathrm{e}^{-\mathrm{i}tH}),$$

would be independent of t and consequently the expectation of the current (140) would be zero. The problem resides in the fact that with the density of fermions being non-zero in the state ω_T^+, the total charge in the reservoir $\mathfrak{R}_k$, $\omega_T^+(\mathrm{d}\Gamma(1_k^{(r)} Q 1_k^{(r)}))$, is actually infinite. Alternatively stated, the operator $T^+(1_k^{(r)} Q 1_k^{(r)})$ is not trace-class.

We can easily resolve the first problem by regularizing the charge Q. For example, by replacing Q with $Q_q \equiv QF(|Q| \le q)$ for a $q > 0$. We shall only consider charges which are temperate according to the following definition.

Definition 6.5 *A charge Q is called temperate if* $\mathrm{Dom}(|H|^\alpha) \subset \mathrm{Dom}(Q)$ *for some* $\alpha > 0$.

We may regularize a temperate charge by a localization in energy. In fact, if Q is a temperate charge, then $Q_\epsilon \equiv Q(1 + \epsilon H^2)^{-\alpha/2}$ is a bounded charge. To resolve the second problem, we regularize the commutator by localizing it with the help of a function $g \in C_0^\infty(\mathbb{R} \setminus \Sigma_H)$. We remark that if $f \in C_0^\infty(\mathbb{R})$ is such that $g(x)f(x) = xg(x)$ for all $x \in \mathbb{R}$, then the expression

$$\Phi_{Q_\epsilon,g,k}^{(r)} \equiv g(H)\mathrm{i}[H, 1_k^{(r)} Q_\epsilon 1_k^{(r)}]g(H) = g(H)\mathrm{i}[f(H), 1_k^{(r)} Q_\epsilon 1_k^{(r)}]g(H),$$

is well-defined: it only involves bounded operators. Furthermore, since $f(H)$ commutes with Q_ϵ, we have

$$\Phi_{Q_\epsilon,g,k}^{(r)} = g(H)\mathrm{i}[f(H), 1_k^{(r)}]Q_\epsilon 1_k^{(r)} g(H) + g(H) 1_k^{(r)} Q_\epsilon \mathrm{i}[f(H), 1_k^{(r)}]g(H),$$

and Lemma 6.2 shows that $\Phi_{Q_\epsilon,g,k}^{(r)}$ is trace-class. The third problem is thus resolved too.

Lemma 6.6 *Under the hypotheses of Lemma 6.2 the regularized current operator of a temperate charge Q*

$$\Phi^{(r)}_{Q_\epsilon,g,k} \equiv g(H)\mathrm{i}[f(H), 1^{(r)}_k Q_\epsilon 1^{(r)}_k] g(H),$$

is trace-class for all $g \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$, $f \in C_0^\infty(\mathbb{R})$, $\epsilon > 0$ and $r \geq 1$.

To formulate the main result of this section, Theorem 6.7 below, we need to introduce the spectral representations of the Hamiltonians $\widetilde{H}_k$. For $k \in \{1, \dots, M\}$ there exists a measurable family $(\mathfrak{h}_k(\varepsilon))_{\varepsilon\in\mathbb{R}}$ of Hilbert spaces and a unitary operator

$$U_k : \widetilde{\mathscr{H}}_{k,\mathrm{ac}} \to \int^\oplus \mathfrak{h}_k(\varepsilon)\,\mathrm{d}\varepsilon, \tag{141}$$

such that $(U_k\widetilde{H}_k u)(\varepsilon) = \varepsilon(U_k u)(\varepsilon)$ for all $u \in \widetilde{\mathscr{H}}_{k,\mathrm{ac}}$. To each operator $B \in \mathscr{B}(\widetilde{\mathscr{H}}_k, \widetilde{\mathscr{H}}_j)$ such that $f(\widetilde{H}_j)B = Bf(\widetilde{H}_k)$ for all bounded measurable function f, the spectral representation (141) associates a measurable family $b(\varepsilon) \in \mathscr{B}(\mathfrak{h}_k(\varepsilon), \mathfrak{h}_j(\varepsilon))$ such that $(U_j Bu)(\varepsilon) = b(\varepsilon)(U_k u)(\varepsilon)$ for all $u \in \widetilde{\mathscr{H}}_{k,\mathrm{ac}}$. We have in particular the following correspondences

$$\begin{aligned} \widetilde{T}_k &\longrightarrow t_k(\varepsilon), \\ \widetilde{Q}_k &\longrightarrow q_k(\varepsilon), \\ \widetilde{P}_k^\pm &\longrightarrow p_k^\pm(\varepsilon), \\ S_{kj} &\longrightarrow s_{kj}(\varepsilon). \end{aligned}$$

Theorem 6.7 *We suppose that Hypotheses (H1)–(H5) are satisfied. Let ω_T^+ be the NESS described by Proposition 5.14 and Q a temperate charge such that*

$$\mathrm{Ran}\,\widetilde{T}_j \subset \mathrm{Dom}|\widetilde{H}_j|^{\nu+\alpha+1}, \qquad \mathrm{Dom}|H|^\alpha \subset \mathrm{Dom}Q.$$

Then, for any sequence $g_n \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$ such that $0 \leq g_n \leq 1$ and $\lim_n g_n(x) = 1$ almost everywhere the limit

$$\omega_T^+(\mathrm{d}\Gamma(\Phi_{Q,k})) \equiv \lim_n \lim_{\epsilon\to 0} \omega_T^+(\mathrm{d}\Gamma(\Phi^{(r)}_{Q_\epsilon,g_n,k})),$$

exists, is independent of $r \geq 0$, and is given by the Landauer-Büttiker formula

$$\omega_T^+(\mathrm{d}\Gamma(\Phi_{Q,k})) = \sum_{j=1}^M \int \mathrm{tr}_{\mathfrak{h}_j(\varepsilon)} \left\{ t_j(\varepsilon) \left(s^*_{jk}(\varepsilon) q_k(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} p_j^-(\varepsilon) q_j(\varepsilon) p_j^-(\varepsilon) \right) \right\} \frac{\mathrm{d}\varepsilon}{2\pi}.$$

We finish this section with an important property of current observables.

Lemma 6.8 *Let T, Q be bounded operators and H a self-adjoint operator on the Hilbert space $\mathscr{H}$. Let f, g be continuous and bounded functions on $\mathbb{R}$ such that $g(H)[f(H), Q]g(H)$ is trace-class. Finally, let P_ε be the orthogonal projection onto the eigenspace of H associated with the eigenvalue ε. Then*

$$\mathrm{tr}\left(P_\varepsilon T P_\varepsilon g(H)[f(H), Q]g(H)\right) = 0.$$

Proof. By using the cyclic property of the trace, we may write

$$\begin{aligned}\operatorname{tr}\left(P_\varepsilon T P_\varepsilon g(H)[f(H),Q]g(H)\right) &= \operatorname{tr}\left(T P_\varepsilon g(H)[f(H),Q]g(H)P_\varepsilon\right)\\ &= g(\varepsilon)^2\operatorname{tr}\left(T P_\varepsilon [f(H),Q]P_\varepsilon\right),\end{aligned}$$

and the result is a consequence of the identity

$$P_\varepsilon[f(H),Q]P_\varepsilon = P_\varepsilon[f(\varepsilon),Q]P_\varepsilon = 0.$$

□

Current observables thus have the property of being insensitive to the contributions of the point spectrum of the Hamiltonian H to the NESS (the second term on the right hand side of (128)). If ω_T^+ is a NESS described by Proposition 5.14 or Theorem 5.15 we have

$$\omega_T^+(\mathrm{d}\Gamma(\Phi^{(r)}_{Q_\epsilon,g,k})) = \omega_{T^+}(\mathrm{d}\Gamma(\Phi^{(r)}_{Q_\epsilon,g,k})) = \operatorname{tr}(T^+\Phi^{(r)}_{Q_\epsilon,g,k}).$$

This last formula is our starting point for the calculation of steady currents. The rest of this section is dedicated to the calculation of the limit

$$\omega_T^+(\mathrm{d}\Gamma(\Phi_{Q,k})) \equiv \lim_{g\to 1}\lim_{\epsilon\to 0}\operatorname{tr}(T^+\Phi^{(r)}_{Q_\epsilon,g,k}),$$

under the hypotheses of Theorem 6.7.

To simplify notation we shall suppose, up to Section 6.7, that the charge Q is bounded and does not require regularization, i.e., we write Q instead of Q_ϵ.

6.4 Equivalence of currents

In the preceding section, we introduced the observables of current. To do this we have localized the charge in the reservoir with the help of operators $1_k^{(r)}$. In this section, we show that it is possible to achieve the same effect by localizing the charge with an appropriate functions of the conjugate operator A_k by exploiting Remark 5.1. Since the propagation of A_k is controlled by the Mourre estimate, this localization method, introduced in [AEGSS] is best adapted to the calculation of steady current by the time-dependent approach which we have adopted.

The following result expresses the fact (obvious from a physical point of view) that in a stationary regime, the total current in a reservoir does not depend on the depth at which we measure it.

Theorem 6.9 *If the hypotheses of Lemma 6.2 hold, and if T is the generator of a gauge invariant quasi-free state on $\mathscr{O}$ which is also τ-invariant then*

$$\operatorname{tr}(T\Phi^{(r)}_{Q,g,k}),$$

is independent of $r \geq 1$.

Proof. For $r, s \geq 1$ we have $\Phi_k^{(r)} - \Phi_k^{(s)} = \Phi_1 + \Phi_2$ with

$$\Phi_1 \equiv g(H)\mathrm{i}[f(H), (1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)}]g(H),$$
$$\Phi_2 \equiv g(H)\mathrm{i}[f(H), 1_k^{(s)}Q(1_k^{(r)} - 1_k^{(s)})]g(H).$$

Lemma 6.2 implies that

$$g(H)f(H)(1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)}g(H), \qquad g(H)(1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)}f(H)g(H),$$

are both trace-class. Φ_1 is thus trace-class and since T and $f(H)$ commute we may write, using the cyclicity of the trace,

$$\begin{aligned}\mathrm{tr}(T\Phi_1) &= \mathrm{itr}(Tg(H)f(H)(1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)} - Tg(H)(1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)}f(H))\\ &= \mathrm{itr}(Tg(H)f(H)(1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)} - Tg(H)f(H)(1_k^{(r)} - 1_k^{(s)})Q1_k^{(r)})\\ &= 0.\end{aligned}$$

In the same way, we show that Φ_2 is trace class and that $\mathrm{tr}(T\Phi_2) = 0$. □

Let $h \in C^\infty(\mathbb{R})$ be such that $0 \leq h \leq 1$ and

$$h(x) = \begin{cases} 0 & \text{if} \quad x < -1;\\ 1 & \text{if} \quad x > 1.\end{cases}$$

For $a \geq 1$ we set $h_\pm^{(a)}(x) \equiv h(\pm x - a)$ and $h^{(a)} \equiv h_-^{(a)} + h_+^{(a)}$. We note that $g^{(a)} = 1 - h^{(a)} \in C_0^\infty(\mathbb{R})$ with $\mathrm{supp}\, g^{(a)} \subset [-a-1, a+1]$ while $\mathrm{supp}\, h^{(a)} \subset \mathbb{R}\setminus]-a+1, a-1[$.

Theorem 6.10 *If Hypotheses (H4) and (H5) are satisfied and $a \geq 1$ then the operator*

$$\Psi_{Q,g,k}^{(a)} \equiv g(H)i[f(H), h^{(a)}(A_k)Qh^{(a)}(A_k)]g(H). \tag{142}$$

is trace-class. Furthermore, if T is the generator of a τ-invariant, gauge invariant, quasi-free state on $\mathcal{O}$ then

$$\mathrm{tr}(T\Psi_{Q,g,k}^{(a)}) = \mathrm{tr}(T\Phi_{Q,g,k}^{(1)}).$$

Proof. We write

$$\Phi_{Q,g,k}^{(1)} = \mathrm{i}[f(H), g(H)1_k(h^{(a)}(A_k) + g^{(a)}(A_k))Q(h^{(a)}(A_k) + g^{(a)}(A_k))1_k g(H)].$$

By Lemma 5.1, $\mathrm{Ran}\,(I - 1_k) \subset \mathrm{Ker}\, A_k$ and since $h^{(a)}(0) = 0$ for $a \geq 1$ one has $h^{(a)}(A_k)(I - 1_k) = (I - 1_k)h^{(a)}(A_k) = 0$. By Lemma 6.3, $g(H)1_k g^{(a)}(A_k)$ is trace-class and we get

$$\Phi_{Q,g,k}^{(1)} = \Psi_{Q,g,k}^{(a)} + [f(H), C],$$

where C is trace-class. Lemma 6.6 thus implies that $\Psi_{Q,g,k}^{(a)}$ is trace-class.

If T commutes with $f(H)$, the cyclic property of the trace implies that

$$\mathrm{tr}(T\Phi^{(1)}_{Q,g,k}) = \mathrm{tr}(T\Psi^{(a)}_{Q,g,k}).$$

□

If the hypotheses of the previous theorem hold, we have

$$\omega_T^+(\mathrm{d}\Gamma(\Phi^{(1)}_{Q,k})) = \lim_{g\to 1}\lim_{\epsilon\to 0}\mathrm{tr}(T^+\Psi^{(a)}_{Q_\epsilon,g,k}), \tag{143}$$

for all $a \geq 1$. The evaluation of the trace on the right hand side of this relation is a difficult problem which is the aim of the two following sections.

6.5 Calculation of steady current I

The first step in the evaluation of the formula (143) is largely inspired by the article of Avron *et al.* [AEGSS]. The idea is to develop the current operator

$$\Psi^{(a)}_{Q,g,k} = \sum_{\sigma,\sigma'\in\{\pm\}} \Psi^{(a,\sigma,\sigma')}_{Q,g,k}, \tag{144}$$

where

$$\Psi^{(a,\sigma,\sigma')}_{Q,g,k} \equiv g(H)i[f(H), h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)]g(H), \tag{145}$$

and to exploit the property of the commutator $[H, h^{(a)}_\sigma(A_k)]$ which appears in this last expression (recall that $f(H)g(H) = Hg(H)$). By expanding this commutator

$$[H, h^{(a)}_\sigma(A_k)] \sim h^{(a)\prime}_\sigma(A_k)[H, A_k],$$

we note that it is localized in a spectral neighborhood of $A_k = \sigma a$ (see Lemma 6.12 below for a precise statement). The Mourre estimate tells us how states in the range of this localized operator propagates,

$$\mathrm{e}^{\mathrm{i}\sigma tH} h^{(a)\prime}_\sigma(A_k) \sim h^{(a)\prime}_\sigma(A_k + \theta t)\mathrm{e}^{\mathrm{i}\sigma tH}.$$

The sample $\mathfrak{S}$ being confined to the the subspace $A_k = 0$ by Hypothesis (H3), we conclude that these states do not undergo scattering when $t \to \sigma\infty$. The Møller operator $\Omega^{\sigma *}$ thus acts trivially on such states, while $\Omega^{-\sigma *} = \Omega^{-\sigma *}\Omega^\sigma\Omega^{\sigma *}$ acts like the scattering matrix $\Omega^{-\sigma *}\Omega^\sigma$.

The result of this first reduction of the problem is the following.

Theorem 6.11 *We suppose that Hypotheses (H1), (H2), (H3), and (H4) are satisfied. Let $\widetilde{T}_j$ be the generator of a τ_j-invariant, gauge invariant, quasi-free state on $\mathcal{O}_j$ such that* $\mathrm{Ran}\,\widetilde{T}_j^{1/2} \subset \mathrm{Dom}\,\widetilde{H}_j$*. For all $g \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$ we have*

$$\lim_{a\to\infty}\Big[\mathrm{tr}(\Omega_j^-\widetilde{T}_j\Omega_j^{-*}\Psi^{(a)}_{Q,g,k}) - \mathrm{tr}\Big(\widetilde{T}_j\Big\{S^*_{jk}\widetilde{\Psi}^{(a,+,+)}_{Q,g,k}S_{kj}$$
$$+\delta_{jk}\Big(\widetilde{P}^-_k\widetilde{\Psi}^{(a,-,-)}_{Q,g,k}\widetilde{P}^-_k + S^*_{kk}\widetilde{\Psi}^{(a,+,-)}_{Q,g,k}\widetilde{P}^-_k + \widetilde{P}^-_k\widetilde{\Psi}^{(a,-,+)}_{Q,g,k}S_{kk}\Big)\Big\}\Big)\Big] = 0. \tag{146}$$

where $\widetilde{\Psi}^{(a,\sigma,\sigma')}_{Q,g,k} \equiv M_k^*\Psi^{(a,\sigma,\sigma')}_{Q,g,k}M_k$.

The main technical tool necessary for the proof of this result is the following localization lemma due to [AEGSS]. Since its proof is quite long, we defer it to Appendix B.

Lemma 6.12 *If Hypotheses (H1), (H2), (H3), and (H4) are satisfied then, for all $f \in C_0^\infty(\mathbb{R})$ and all $g \in C_0^\infty(\mathbb{R} \setminus \Sigma_H)$:*

(i) $\sup_{a\ge 1} \|[f(H), h_\pm^{(a)}(A_k)]g(H)\|_1 < \infty$.

(ii) There exist constants $s > 1$ and C such that, for all $a, \alpha \ge 1$,

$$\|F(\pm A < a - \alpha)[f(H), h_\pm^{(a)}(A_k)]g(H)\|_1 < C\langle\alpha\rangle^{-s}.$$

Remark. It follows from (i) that the components $\Psi_{Q,g,k}^{(a,\sigma,\sigma')}$ of the current are trace-class operators.

To prepare for the proof of Theorem 6.11 we begin by proving the following lemma.

Lemma 6.13 *We suppose that the hypotheses of Theorem 6.11 are satisfied. For $\alpha \in \{j, l\} \subset \{1, \dots, M\}$ let $\widetilde{T}_\alpha$ be the generator of a τ_α-invariant, gauge invariant, quasi-free state on $\mathcal{O}_\alpha$ such that* $\operatorname{Ran} \widetilde{T}_\alpha^{1/2} \subset \operatorname{Dom} \widetilde{H}_\alpha$. *For all $g \in C_0^\infty(\mathbb{R} \setminus \Sigma_H)$ we have:*

$$\lim_{a\to\infty} \|\widetilde{T}_j^{1/2}(\Omega_j^{\sigma*}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}\Omega_l^{\sigma'} - \delta_{jk}M_k^*\Psi_{Q,g,k}^{(a,\sigma,\sigma')}M_k\delta_{kl})\widetilde{T}_l^{1/2}\|_1 = 0. \tag{147}$$

Proof. Since Q commutes with $f(H)$, we may write

$$\begin{aligned}\Psi_{Q,g,k}^{(a,\sigma,\sigma')} &= g(H)\mathrm{i}[f(H), h_\sigma^{(a)}(A_k)]Qh_{\sigma'}^{(a)}(A_k)g(H)\\ &\quad + g(H)h_\sigma^{(a)}(A_k)Q\mathrm{i}[f(H), h_{\sigma'}^{(a)}(A_k)]g(H).\end{aligned} \tag{148}$$

Q being bounded, this decomposition, the inequality $\|BC\|_1 \le \|B\|\,\|C\|_1$, and a telescopic expansion allow us to reduce the proof to the following three assertions

$$\sup_{a\ge 1} \|g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 < \infty, \tag{149}$$

$$\lim_{a\to\infty} \|\widetilde{T}_j^{1/2}(\Omega_j^{\sigma*} - \delta_{jk}M_j^*)g(H)h_\sigma^{(a)}(A_k)\| = 0, \tag{150}$$

$$\lim_{a\to\infty} \|\widetilde{T}_j^{1/2}(\Omega_j^{\sigma*} - \delta_{jk}M_j^*)g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 = 0. \tag{151}$$

We immediately remark that (149) follows from Assertion (i) of Lemma 6.12 by taking the adjoint.

Hypothesis (H2) (ii) (iv) allows us to write

$$(HM_j - M_j\widetilde{H}_j)\widetilde{T}_j^{1/2} = J_j[\widetilde{H}_j, \widetilde{\chi}_j]\widetilde{T}_j^{1/2} = J_jB_j\widetilde{T}_j^{1/2},$$

and to conclude that $(HM_j - M_j\widetilde{H}_j)\widetilde{T}_j^{1/2}$ is bounded. We now remark that first, the identity (123) implies

$$\operatorname{Ran}(HM_j - M_j\widetilde{H}_j)\widetilde{T}_j^{1/2} \subset \operatorname{Ker} A_j,$$

and second, Hypothesis (H1) (iii) shows that, for $k \neq j$,

$$1_k (HM_j - M_j \widetilde{H}_j)\widetilde{T}_j = 1_k J_j [\widetilde{H}_j, \widetilde{\chi}_j]\widetilde{T}_j^{1/2} = 0.$$

Since $A = \sum_{k=1}^{M} A_k 1_k$ we get that

$$\mathrm{Ran}\,(HM_j - M_j \widetilde{H}_j)\widetilde{T}_j^{1/2} \subset \mathrm{Ker}\, A,$$

and that, consequently,

$$(HM_j - M_j \widetilde{H}_j)\widetilde{T}_j^{1/2} = F(\sigma A \le \vartheta t + a/2 - 1)(HM_j - M_j \widetilde{H}_j)\widetilde{T}_j^{1/2}, \tag{152}$$

for all $\vartheta t \ge 0$ and $a \ge 2$.

The adjoint of this last relation and the fact that $\widetilde{T}_j$ and $\mathrm{e}^{\mathrm{i}t\widetilde{H}_j}$ commute allow us to write the Cook representation

$$\begin{aligned} &\widetilde{T}_j^{1/2}(\Omega_j^{\sigma *} - M_j^*)g(H)h_\sigma^{(a)}(A_k) = \\ &\qquad \mathrm{i}\sigma \int_0^\infty \mathrm{e}^{\mathrm{i}\sigma t \widetilde{H}_j}\widetilde{T}_j^{1/2}(\widetilde{H}_j M_j^* - M_j^* H)F(\sigma A \le \vartheta t + a/2 - 1)\mathrm{e}^{-\mathrm{i}\sigma t H} g(H) h_\sigma^{(a)}(A_k)\,\mathrm{d}t, \end{aligned} \tag{153}$$

valid for all $\vartheta > 0$. By invoking the fact that $A = \oplus_{k=1}^{M} A_k$, it follows from the definition of the functions $h_\pm^{(a)}$ that

$$h_\sigma^{(a)}(A_k) = F(\sigma A \ge a - 1)h_\sigma^{(a)}(A_k),$$

which allows us to write, with $a' = a - 1$,

$$\|F(\sigma A \le \vartheta t + a/2 - 1)\mathrm{e}^{-\mathrm{i}\sigma t H} g(H) h_\sigma^{(a)}(A_k)\| \le \|F(\sigma A \le a' - a/2 + \vartheta t)\mathrm{e}^{-\mathrm{i}\sigma t H} g(H) F(\sigma A \ge a')\|.$$

By Hypothesis (H4) (ii), Assertion (ii) of Theorem 5.2 and Proposition 4.27 it is possible to choose $\vartheta > 0$ in such a way that there exists a constant C_1 such that

$$\|F(\sigma A \le \vartheta t + a/2 - 1)\mathrm{e}^{-\mathrm{i}\sigma t H} g(H) h_\sigma^{(a)}(A_k)\| \le C_1 \langle a/2 + \vartheta t\rangle^{-s}, \tag{154}$$

for some $s > 1$ and for all $a \ge 2$, $t \ge 0$. With the representation (153) we obtain

$$\|\widetilde{T}_j^{1/2}(\Omega_j^{\sigma *} - M_j^*)g(H)h_\sigma^{(a)}(A_k)\| \le \|\widetilde{T}_j^{1/2}(\widetilde{H}_j M_j^* - M_j^* H)\| \int_0^\infty C_1 \langle a/2 + \vartheta t\rangle^{-s}\,\mathrm{d}s,$$

and if $j = k$, (150) follows from an dominated convergence argument. To finish the proof of (150), it suffices to show that

$$\lim_{a\to\infty} \|M_j^* g(H) h_\sigma^{(a)}(A_k)\| = 0,$$

when $j \neq k$. To do this we begin by remarking that $A_k 1_j = 0$ and thus $\mathrm{Ran}\, M_j \subset \mathrm{Ker}\, A_k$. We get that

$$\begin{aligned} \|M_j^* g(H) h_\sigma^{(a)}(A_k)\| &= \|M_j^* F(A_k = 0) g(H) h_\sigma^{(a)}(A_k)\| \\ &\le \|F(A_k = 0) g(H) h_\sigma^{(a)}(A_k)\| \\ &\le \|1_k F(A = 0) g(H) h_\sigma^{(a)}(A_k)\| \\ &\le \|F(\sigma A \le a/2 - 1) g(H) h_\sigma^{(a)}(A_k)\|, \end{aligned} \tag{155}$$

for $a \geq 2$. The estimate (154), with $t = 0$ allows us to conclude.

By proceeding in a similar way we obtain the Cook representation

$$\widetilde{T}_j^{1/2}(\Omega_j^{\sigma *} - M_j^*) g(H)[f(H), h_\sigma^{(a)}(A_k)] = \mathrm{i}\sigma \int_0^\infty \mathrm{e}^{\mathrm{i}\sigma t \widetilde{H}_j} \widetilde{T}_j^{1/2}(\widetilde{H}_j M_j^* - M_j^* H) \\ \times F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H)[f(H), h_\sigma^{(a)}(A_k)] g(H) \,\mathrm{d}t, \tag{156}$$

valid for all $\vartheta > 0$. To estimate the integral of the right hand side of this identity, we decompose

$$F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H)[f(H), h_\sigma^{(a)}(A_k)] g(H) = \\ F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H) F(\sigma A \geq (a - \vartheta t)/2)[f(H), h_\sigma^{(a)}(A_k)] g(H) \\ + F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H) F(\sigma A < (a - \vartheta t)/2)[f(H), h_\sigma^{(a)}(A_k)] g(H),$$

and thus obtain

$$\|F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H)[f(H), h_\sigma^{(a)}(A_k)] g(H)\|_1 \leq \\ \|F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H) F(\sigma A \geq (a - \vartheta t)/2)\| \, \|[f(H), h_\sigma^{(a)}(A_k)] g(H)\|_1 \\ + \|F(\sigma A < (a - \vartheta t)/2)[f(H), h_\sigma^{(a)}(A_k)] g(H)\|_1, \tag{157}$$

We consider the first term on the right hand side of this inequality. Its second factor is uniformly bounded by (i) of Lemma 6.12. By setting $a' = (a - \vartheta t)/2$ its first factor can be written as

$$\|F(\sigma A \leq a' - a/2 + \vartheta t) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H) F(\sigma A \geq a')\|.$$

As before, we invoke Assertion (ii) of Theorem 5.2 and Proposition 4.27 to choose $\vartheta > 0$ so that this factor is bounded by $C_1 \langle a/2 + \vartheta t \rangle^{-s}$.

Writing the second term on the right hand side of (157) as

$$\|F(\sigma A < a - (a + \vartheta t)/2)[f(H), h_\sigma^{(a)}(A_k)] g(H)\|_1,$$

Assertion (ii) of Lemma 6.12 allows us to conclude that it is bounded by $C\langle a/2 + \vartheta t/2\rangle^{-s}$ for a constant C and some $s > 1$. We have thus shown that

$$\|F(\sigma A \leq \vartheta t/2) \mathrm{e}^{-\mathrm{i}\sigma t H} g(H)[f(H), h_\sigma^{(a)}(A_k)] g(H)\|_1 \leq C_2 \langle a + \vartheta t \rangle^{-s},$$

for a constant C_2, some $s > 1$, and for all $a \geq 2$. For $j = k$, Assertion (151) is an immediate consequence of this estimate and the representation (156). To finish the proof of (151) it suffices to show that

$$\lim_{a \to \infty} \|M_j^* g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 = 0,$$

when $j \neq k$. We proceed as in (155) to obtain

$$\begin{aligned} \|M_j^* g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 &= \|M_j^* F(A_k = 0) g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 \\ &\leq \|F(A_k = 0) g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 \\ &\leq \|1_k F(A = 0) g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1 \\ &\leq \|F(\sigma A < a/2) g(H)[f(H), h_\sigma^{(a)}(A_k)]\|_1, \end{aligned}$$

and we conclude by once again invoking (ii) of Lemma 6.12. □

Proof of Theorem 6.11. We write $C \sim D$ whenever C and D are operators depending on a and such that $\lim_{a\to\infty} \|\widetilde{T}_j^{1/2}(C-D)\widetilde{T}_j^{1/2}\|_1 = 0$ holds.
By invoking Corollary 5.12, we may write

$$\Omega_j^{-*}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}\Omega_j^{-} = \sum_{m,n=1}^{M}\Omega_j^{-*}P_m^{\sigma}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}P_n^{\sigma'}\Omega_j^{-} = \sum_{m,n=1}^{M}\Omega_j^{-*}\Omega_m^{\sigma}\Omega_m^{\sigma*}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}\Omega_n^{\sigma'}\Omega_n^{\sigma'*}\Omega_j^{-}.$$

The properties of the Møller operators show that

$$\Omega_\alpha^{\sigma*}\Omega_j^{-}\mathrm{Dom}\widetilde{H}_j \subset \mathrm{Dom}\widetilde{H}_\alpha.$$

We may thus invoke Lemma 6.13 to continue with

$$\Omega_j^{-*}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}\Omega_j^{-} \sim \Omega_j^{-*}\Omega_k^{\sigma}M_k^{*}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}M_k\Omega_k^{\sigma'*}\Omega_j^{-}.$$

Since

$$\Omega_k^{\sigma*}\Omega_j^{\sigma'} = \begin{cases} S_{kj} & \text{if} \quad \sigma=+ \text{ and } \sigma'=-; \\ \delta_{kj}\widetilde{P}_j^{\sigma} & \text{if} \quad \sigma=\sigma'; \\ S_{kj}^{*} & \text{if} \quad \sigma=- \text{ and } \sigma'=+; \end{cases}$$

we obtain

$$\begin{aligned}\Omega_j^{-*}\Psi_{Q,g,k}^{(a)}\Omega_j^{-} &= \sum_{\sigma,\sigma'\in\{\pm\}}\Omega_j^{-*}\Psi_{Q,g,k}^{(a,\sigma,\sigma')}\Omega_j^{-} \\ &\sim S_{jk}^{*}M_k^{*}\Psi_{Q,g,k}^{(a,+,+)}M_kS_{kj} \\ &+\delta_{kj}\left(S_{kk}^{*}M_k^{*}\Psi_{Q,g,k}^{(a,+,-)}M_k\widetilde{P}_k^{-}+\widetilde{P}_k^{-}M_k^{*}\Psi_{Q,g,k}^{(a,-,+)}M_kS_{kk}+\widetilde{P}_k^{-}M_k^{*}\Psi_{Q,g,k}^{(a,-,-)}M_k\widetilde{P}_k^{-}\right).\end{aligned}$$

□

6.6 Calculation of steady current II

In this section we finish the calculation of the steady current starting from the formula (146). The method which we use here differs from that of [AEGSS]. In fact, in this work the reservoirs are straight, one-dimensional wires without internal structure. In this case we may choose the conjugate operator in such a way that $\mathrm{i}[\widetilde{H}_k,\widetilde{A}_k] = 2\widetilde{H}_k$ and it is easy to explicitly construct the spectral representations of $\widetilde{H}_k$ and $\widetilde{A}_k$ and to compute the integral kernel of operators of the form $f(\widetilde{H}_k)g(\widetilde{A}_k)$. This reduces the calculation of their trace to an integral over the diagonal of this integral kernel. This approach is inapplicable at the level of generality where we have placed ourselves. We shall use a more systematic approach based uniquely on the propagation estimates and on the abstract spectral representation of the operator $\widetilde{H}_k$.

6.6.1 Preliminaries

We begin by showing that it is possible to replace H with $\widetilde{H}_k$ and A_k by $\widetilde{A}_k$ in the definition of $\widetilde{\Psi}^{(a,\sigma,\sigma')}_{Q,g,k}$ without altering its NESS expectation.

Lemma 6.14 *Under Hypothesis (H5) we have*

$$\lim_{a\to\infty}\left\|\widetilde{\Psi}^{(a,\sigma,\sigma')}_{Q,g,k}-\widetilde{\Psi}^{\#(a,\sigma,\sigma')}_{Q,g,k}\right\|_1=0.$$

where $\widetilde{\Psi}^{\#(a,\sigma,\sigma')}_{Q,g,k}\equiv g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k),h^{(a)}_\sigma(\widetilde{A}_k)M_k^*QM_kh^{(a)}_{\sigma'}(\widetilde{A}_k)]g(\widetilde{H}_k)$.

Proof. We shall write $C\sim D$ when $\lim_{a\to\infty}\|C-D\|_1=0$. By Lemma 6.1, $M_k^*g(H)-g(\widetilde{H}_k)M_k^*$ and $g(H)M_k-M_kg(\widetilde{H}_k)$ are trace-class. Since

$$\mathrm{s}^*-\lim_{a\to\infty}h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)=0,$$

we have

$$M_k^*g(H)\mathrm{i}[f(H),h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)]g(H)M_k\sim g(\widetilde{H}_k)M_k^*\mathrm{i}[f(H),h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)]M_kg(\widetilde{H}_k).$$

We prove in the same way that

$$g(\widetilde{H}_k)M_k^*\mathrm{i}[f(H),h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)]M_kg(\widetilde{H}_k)\sim g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k),M_k^*h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)M_k]g(\widetilde{H}_k).$$

Finally, it follows from the identity (135) that

$$M_k^*h^{(a)}_\sigma(A_k)=M_k^*M_kh^{(a)}_\sigma(\widetilde{A}_k)M_k^*=1_kh^{(a)}_\sigma(\widetilde{A}_k)M_k^*=h^{(a)}_\sigma(\widetilde{A}_k)M_k^*,$$

from which it follows that

$$g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k),M_k^*h^{(a)}_\sigma(A_k)Qh^{(a)}_{\sigma'}(A_k)M_k]g(\widetilde{H}_k)=g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k),h^{(a)}_\sigma(\widetilde{A}_k)M_k^*QM_kh^{(a)}_{\sigma'}(\widetilde{A}_k)]g(\widetilde{H}_k).$$

□

Corollary 6.15 *Under the hypotheses of Theorem 6.11 and Hypothesis (H5) we have*

$$\begin{aligned}\mathrm{tr}(\Omega_j^-\widetilde{T}_j\Omega_j^{-*}\Psi^{(a)}_{Q,g,k})=\mathrm{tr}\Big(\widetilde{T}_j\Big\{&S_{jk}^*\widetilde{\Psi}^{\#(a,+,+)}_{Q,g,k}S_{kj}\\ +\delta_{jk}\Big(&\widetilde{P}_k^-\widetilde{\Psi}^{\#(a,-,-)}_{Q,g,k}\widetilde{P}_k^-+S_{kk}^*\widetilde{\Psi}^{\#(a,+,-)}_{Q,g,k}\widetilde{P}_k^-+\widetilde{P}_k^-\widetilde{\Psi}^{\#(a,-,+)}_{Q,g,k}S_{kk}\Big)\Big\}\Big).\end{aligned}\tag{158}$$

for all $a\geq 1$.

Proof. Since $\Omega_j^-\widetilde{T}_j\Omega_j^{-*}$ commutes with H, Theorem 6.10 shows that the left hand side of (158) is independent of $a\geq 1$. By taking into account Proposition 6.11 and Lemma 6.14, it suffices to show that that the right hand side is also independent of a.

For $a, b \geq 1$, we have $g_\sigma \equiv h_\sigma^{(a)} - h_\sigma^{(b)} \in C_0^\infty(\mathbb{R})$. It follows from Hypothesis (H4) (i) that $C_\sigma \equiv g(\widetilde{H}_k) g_\sigma(\widetilde{A}_k) = g(\widetilde{H}_k)(\widetilde{A}_k + \mathrm{i})^{-m}(\widetilde{A}_k + \mathrm{i})^m g_\sigma(\widetilde{A}_k)$ is trace-class. Since

$$\begin{aligned}\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} - \widetilde{\Psi}_{Q,g,k}^{\#(b,\sigma,\sigma')} &= \mathrm{i}[f(\widetilde{H}_k), C_\sigma M_k^* Q M_k h_{\sigma'}^{(a)}(\widetilde{A}_k) g(\widetilde{H}_k)] \\ &\quad + \mathrm{i}[f(\widetilde{H}_k), g(\widetilde{H}_k) h_\sigma^{(b)}(\widetilde{A}_k) M_k^* Q M_k C_{\sigma'}^*],\end{aligned}$$

and $S_{kj}\widetilde{T}_j S_{jk}^*$ commutes with $\widetilde{H}_k$ the cyclic property of the trace allows us to conclude that

$$\operatorname{tr}\left(S_{kj}\widetilde{T}_j S_{jk}^*\left(\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} - \widetilde{\Psi}_{Q,g,k}^{\#(b,\sigma,\sigma')}\right)\right) = 0.$$

The 3 other terms of the right hand side of (158) are treated in a similar manner. □

6.6.2 Spectral representation of the current

We are now in position to pass to the spectral representation (141).

The main result of this section is the following.

Theorem 6.16 *We suppose that Hypotheses (H1), (H2) and (H3) are satisfied. If $g \in C_0^\infty(\mathbb{R} \setminus \Sigma_H)$ and if the operator*

$$\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} = g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k), h_\sigma^{(a)}(\widetilde{A}_k) M_k^* Q M_k h_{\sigma'}^{(a)}(\widetilde{A}_k)] g(\widetilde{H}_k),$$

is trace-class, then:

(i) $\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')}$ *reduces to its part in $\widetilde{\mathcal{H}}_{k,\mathrm{ac}}$, that is to say that*

$$\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} = P_{\mathrm{ac}}(\widetilde{H}_k)\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} P_{\mathrm{ac}}(\widetilde{H}_k).$$

(ii) There exists a measurable set $\Delta \subset \mathbb{R}$, with $\mathbb{R} \setminus \Delta$ having Lebesgue measure zero, and a mapping

$$\Delta \times \Delta \ni \langle \varepsilon, \varepsilon' \rangle \mapsto \psi_{Q,g,k}^{\#(a,\sigma,\sigma')}(\varepsilon', \varepsilon) \in \mathcal{L}^1(\mathfrak{h}_k(\varepsilon), \mathfrak{h}_k(\varepsilon')),$$

such that, for all $u, v \in \widetilde{\mathcal{H}}_{k,\mathrm{ac}}$,

$$(u, \widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} v) = \int ((U_k u)(\varepsilon'), \psi_{Q,g,k}^{\#(a,\sigma,\sigma')}(\varepsilon', \varepsilon)(U_k v)(\varepsilon))_{\mathfrak{h}_k(\varepsilon')} \mathrm{d}\varepsilon \mathrm{d}\varepsilon',$$

(iii) For all $\varepsilon \in \Delta$,

$$\psi_{Q,g,k}^{\#(a,\sigma,\sigma')}(\varepsilon, \varepsilon) = \frac{\sigma}{2\pi} g(\varepsilon)^2 p_k^\sigma(\varepsilon) q_k(\varepsilon) p_k^\sigma(\varepsilon) \delta_{\sigma\sigma'}. \tag{159}$$

We shall show in Section 6.7 how Formula (159) can be used to complete the calculation of the steady current. The rest of this section is dedicated to the proof of Theorem 6.16 which is organized as follows. In Section 6.6.3 we prove a theorem about the general structure of trace-class operators on a direct integral of Hilbert spaces and in particular the existence of the integral kernel of such an operator. In Section 6.6.4 we show how to compute the diagonal of this integral kernel. These results allow us finally to prove Theorem 6.16 in Section 6.6.5.

6.6.3 Trace-class operators on $\int^{\oplus} \mathfrak{h}_\varepsilon \mathrm{d}\mu(\varepsilon)$

Theorem 6.17 *Let $\Delta \subset \mathbb{R}$ be a measurable set, μ a σ-finite measure on Δ and $(\mathfrak{h}_\varepsilon)_{\varepsilon\in\Delta}$ a family of μ-measurable, separable Hilbert spaces. If C is a trace-class operator on $\mathfrak{H} \equiv \int_\Delta^{\oplus} \mathfrak{h}_\varepsilon \,\mathrm{d}\mu(\varepsilon)$ then:*

(i) There exists a measurable set $\Delta_0 \subset \Delta$ such that $\Delta \setminus \Delta_0$ is μ-negligible and, for all $\langle \varepsilon', \varepsilon\rangle \in \Delta_0 \times \Delta_0$, a trace-class operator $c(\varepsilon',\varepsilon) : \mathfrak{h}_\varepsilon \to \mathfrak{h}_{\varepsilon'}$ such that $\langle \varepsilon',\varepsilon\rangle \mapsto (u(\varepsilon'), c(\varepsilon',\varepsilon)v(\varepsilon))_{\mathfrak{h}_{\varepsilon'}}$ is measurable for all $u, v \in \mathfrak{H}$.

(ii) For all $u, v \in \mathfrak{H}$, $(u, Cv) = \int_\Delta (u(\varepsilon'), c(\varepsilon',\varepsilon)v(\varepsilon))_{\mathfrak{h}_{\varepsilon'}} \mathrm{d}\mu(\varepsilon)\mathrm{d}\mu(\varepsilon')$.

(iii) $\int_\Delta \|c(\varepsilon,\varepsilon)\|_1 \,\mathrm{d}\mu(\varepsilon) \le \|C\|_1$.

(iv) $\int_\Delta \mathrm{tr}_{\mathfrak{h}_\varepsilon}(c(\varepsilon,\varepsilon))\,\mathrm{d}\mu(\varepsilon) = \mathrm{tr}(C)$.

Since this result does not seem to be widely known, we give a proof by following [Y].

Proof. C being compact, it admits a canonical representation

$$C = \sum_{n\in N} \kappa_n u_n^+(u_n^-, \cdot),$$

where N is a set which is at most countable, $(u_n^\pm)_{n\in N}$ are orthonormal families in $\mathfrak{H}$, and $(\kappa_n)_{n\in N}$ is the family of singular values of C. In particular we have $\kappa_n > 0$ and $\sum_{n\in N}\kappa_n = \|C\|_1 < \infty$. Since

$$\|C\|_1 = \sum_{n\in N} \kappa_n \int_\Delta \|u_n^\pm(\varepsilon)\|^2_{\mathfrak{h}_\varepsilon} \mathrm{d}\mu(\varepsilon) < \infty,$$

Fubini's theorem implies the existence of a measurable set $\Delta^\pm \subset \Delta$, such that $\Delta\setminus\Delta^\pm$ is μ-negligible and $\sum_{n\in N}\kappa_n\|u_n^\pm(\varepsilon)\|^2_{\mathfrak{h}_\varepsilon} < \infty$ for all $\varepsilon\in\Delta^\pm$. We set $\Delta_0 \equiv \Delta^+ \cap \Delta^-$. $\Delta\setminus\Delta_0$ is μ-negligible and, for all $\varepsilon, \varepsilon' \in \Delta_0$,

$$c(\varepsilon',\varepsilon) \equiv \sum_{n\in N} \kappa_n u_n^+(\varepsilon')(u_n^-(\varepsilon), \cdot)_{\mathfrak{h}_\varepsilon},$$

converges in norm in $\mathscr{B}(\mathfrak{h}_\varepsilon, \mathfrak{h}_{\varepsilon'})$. In fact, the Cauchy-Schwarz inequality implies

$$\sum_{n\in N} \kappa_n \|u_n^+(\varepsilon')\|_{\mathfrak{h}_{\varepsilon'}} \|u_n^-(\varepsilon)\|_{\mathfrak{h}_\varepsilon} \le \left(\sum_{n\in N}\kappa_n\|u_n^+(\varepsilon')\|^2_{\mathfrak{h}_{\varepsilon'}} \sum_{m\in N}\kappa_m \|u_m^-(\varepsilon)\|^2_{\mathfrak{h}_\varepsilon}\right)^{1/2} < \infty.$$

For $u, v \in \mathfrak{H}$ we thus have

$$\begin{aligned}\int_\Delta (u(\varepsilon'), c(\varepsilon',\varepsilon)v(\varepsilon))_{\mathfrak{h}_{\varepsilon'}} \mathrm{d}\mu(\varepsilon)\mathrm{d}\mu(\varepsilon') &= \sum_{n\in N}\kappa_n \int_\Delta (u(\varepsilon'), u_n^+(\varepsilon'))_{\mathfrak{h}_{\varepsilon'}} \mathrm{d}\mu(\varepsilon') \int_\Delta (u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon} \mathrm{d}\mu(\varepsilon) \\ &= \sum_{n\in N}\kappa_n (u, u_n^+)(u_n^-, v) = (u, Cv).\end{aligned}$$

Since $\|u_n^+(\varepsilon)(u_n^-(\varepsilon),\cdot)_{\mathfrak{h}_\varepsilon}\|_1 = \|u_n^+(\varepsilon)\|_{\mathfrak{h}_\varepsilon}\|u_n^-(\varepsilon)\|_{\mathfrak{h}_\varepsilon}$ we have

$$\begin{aligned}\int_\Delta \|c(\varepsilon,\varepsilon)\|_1\,\mathrm{d}\mu(\varepsilon) &\le \sum_{n\in N}\kappa_n\int_\Delta \|u_n^+(\varepsilon)\|_{\mathfrak{h}_\varepsilon}\|u_n^-(\varepsilon)\|_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\mu(\varepsilon)\\ &\le \sum_{n\in N}\kappa_n\left(\int_\Delta \|u_n^+(\varepsilon)\|^2_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\mu(\varepsilon)\int_\Delta \|u_n^-(\varepsilon')\|^2_{\mathfrak{h}_{\varepsilon'}}\,\mathrm{d}\mu(\varepsilon')\right)^{1/2}\\ &= \sum_{n\in N}\kappa_n\|u_n^+\|\,\|u_n^-\|\\ &= \sum_{n\in N}\kappa_n = \|C\|_1.\end{aligned}$$

Similarly, since $\mathrm{tr}(u_n^+(\varepsilon)(u_n^-(\varepsilon),\cdot))_{\mathfrak{h}_\varepsilon} = (u_n^-(\varepsilon),u_n^+(\varepsilon))_{\mathfrak{h}_\varepsilon}$,

$$\int_\Delta \mathrm{tr}(c(\varepsilon,\varepsilon))\,\mathrm{d}\mu(\varepsilon) = \sum_{n\in N}\kappa_n\int_\Delta (u_n^-(\varepsilon),u_n^+(\varepsilon))_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\mu(\varepsilon) = \sum_{n\in N}\kappa_n(u_n^-,u_n^+) = \mathrm{tr}(C).$$

□

To compare the operators in a direct sum of Hilbert spaces, the following result is also useful.

Lemma 6.18 *Let $\Delta\subset\mathbb{R}$ be a measurable set equipped with a σ-finite measure μ, $(\mathfrak{h}_\varepsilon)_{\varepsilon\in\Delta}$ a family of μ-measurable, separable Hilbert spaces, and $\mathscr{D}\subset\mathfrak{H}\equiv\int_\Delta^\oplus \mathfrak{h}_\varepsilon\,\mathrm{d}\mu(\varepsilon)$ a dense subspace. If $\Delta\ni\varepsilon\mapsto a(\varepsilon)\in\mathscr{B}(\mathfrak{h}_\varepsilon)$ is a mapping such that, for all $u,v\in\mathscr{D}$, there exists a μ-negligible set $\Delta_{uv}\subset\Delta$ with the property that*

$$(u(\varepsilon),a(\varepsilon)v(\varepsilon))_{\mathfrak{h}_\varepsilon} = 0,$$

for all $\varepsilon\in\Delta\setminus\Delta_{uv}$, then $a(\varepsilon)=0$ for μ-almost every $\varepsilon\in\Delta$.

Proof. Since $\mathfrak{H}$ is separable it is possible to extract a countable family $(u_n)_{n\in N}\subset\mathscr{D}$ which is dense. For each $n\in N$, let Δ_n be the set of $\varepsilon\in\Delta$ for which $u_n(\varepsilon)\in\mathfrak{h}_\varepsilon$ is defined. Then $\Delta\setminus\Delta_n$ is μ-negligible and the same is true of $\Delta\setminus\tilde\Delta$ where $\tilde\Delta\equiv\cap_{n\in N}\Delta_n$.

For all $\varepsilon\in\tilde\Delta$, we may apply to the family $(u_n(\varepsilon))_{n\in N}$ the Gramm-Schmidt procedure to obtain an orthonormal basis $(g_m(\varepsilon))_{m\in M}$ of the closed subspace $\mathfrak{u}_\varepsilon\subset\mathfrak{h}_\varepsilon$ generated by $(u_n(\varepsilon))_{n\in N}$. For all $m\in M$ we have $g_m(\varepsilon)=\sum_{n\in N}\alpha_{mn}(\varepsilon)u_n(\varepsilon)$, this sum being finite (i.e., $\{n\in N\,|\,\alpha_{mn}(\varepsilon)\neq 0\}$ is finite for all $m\in M$). Furthermore each coefficient $\alpha_{mn}(\varepsilon)$ is a measurable function of a finite number of scalar products $(u_i(\varepsilon),u_j(\varepsilon))_{\mathfrak{h}_\varepsilon}$ which are measurable functions of ε. We conclude that for all $u\in\mathfrak{H}$ the functions $\tilde\Delta\ni\varepsilon\mapsto(g_m(\varepsilon),u(\varepsilon))_{\mathfrak{h}_\varepsilon}$ are measurable. Let $p(\varepsilon)$ be the orthogonal projection onto $\mathfrak{u}_\varepsilon$. The Cauchy-Schwarz and Bessel inequalities show that for all $u,v\in\mathfrak{H}$ and for all $\varepsilon\in\tilde\Delta$ for which $u(\varepsilon)$ and $v(\varepsilon)$ are defined, the series

$$(u(\varepsilon),p(\varepsilon)v(\varepsilon))_{\mathfrak{h}_\varepsilon} = \sum_{m\in M}(u(\varepsilon),g_m(\varepsilon))_{\mathfrak{h}_\varepsilon}(g_m(\varepsilon),v(\varepsilon))_{\mathfrak{h}_\varepsilon},$$

converges absolutely. Its sum is thus a measurable function defined μ-almost everywhere which satisfies

$$\left|\sum_{m\in M}(u(\varepsilon),g_m(\varepsilon))_{\mathfrak{h}_\varepsilon}(g_m(\varepsilon),v(\varepsilon))_{\mathfrak{h}_\varepsilon}\right| \le \|u(\varepsilon)\|_{\mathfrak{h}_\varepsilon}\|v(\varepsilon)\|_{\mathfrak{h}_\varepsilon}.$$

The Cauchy-Schwarz inequality and Fubini's theorem allow us to conclude that

$$(u, Pv) \equiv \int (u(\varepsilon), p(\varepsilon)v(\varepsilon))_{\mathfrak{h}_\varepsilon} \, \mathrm{d}\varepsilon,$$

defines a bounded operator on $\mathfrak{H}$. By construction, $Pu_n = u_n$ for all $n \in N$. Since $(u_n)_{n\in N}$ is dense in $\mathfrak{H}$, it follows that $P = I$ and consequently,

$$0 = (u, (I-P)u) = \int (u(\varepsilon), (I-p(\varepsilon))u(\varepsilon))_{\mathfrak{h}_\varepsilon} \, \mathrm{d}\varepsilon, = \int \|(I-p(\varepsilon))u(\varepsilon)\|^2_{\mathfrak{h}_\varepsilon} \, \mathrm{d}\varepsilon,$$

for all $u \in \mathfrak{H}$. This implies that $\|(I-p(\varepsilon))u(\varepsilon)\|_{\mathfrak{h}_\varepsilon} = 0$, μ-almost everywhere, that is to say that there exists a measurable set $\tilde{\Delta}_0 \subset \tilde{\Delta}$ such that $\Delta \setminus \tilde{\Delta}_0$ is μ-negligible and $(u_n(\varepsilon))_{n\in N}$ is total in $\mathfrak{h}_\varepsilon$ for all $\varepsilon \in \tilde{\Delta}_0$.

Let

$$\Delta_0 \equiv \left(\bigcap_{n,m\in N} \Delta \setminus \Delta_{u_n u_m} \right) \bigcap \tilde{\Delta}_0.$$

We may conclude the proof of the lemma by remarking that $\Delta \setminus \Delta_0$ is μ-negligible and that for $\varepsilon \in \Delta_0$ we have $(u_n(\varepsilon), a(\varepsilon), u_m(\varepsilon))_{\mathfrak{h}_\varepsilon} = 0$ for all $n, m \in N$ and thus $a(\varepsilon) = 0$. □

6.6.4 The diagonal

The diagonal $c(\varepsilon, \varepsilon)$ of the integral kernel of a trace-class operator C on the Lebesgue direct integral $\int^\oplus \mathfrak{h}_\varepsilon \, \mathrm{d}\varepsilon$ is defined almost everywhere. To calculate this diagonal, the following result is often useful.

Lemma 6.19 *Let $\Delta \subset \mathbb{R}$ be a measurable set and $(\mathfrak{h}_\varepsilon)_{\varepsilon\in\Delta}$ a family of Lebesgue-measurable Hilbert spaces. Let E be the self-adjoint operator on $\mathfrak{H} \equiv \int^\oplus_\Delta \mathfrak{h}_\varepsilon \, \mathrm{d}\varepsilon$ defined by $(Eu)(\varepsilon) = \varepsilon u(\varepsilon)$. If $C \in \mathscr{L}^1(\mathfrak{H})$ and $c(\varepsilon', \varepsilon)$ denotes its integral kernel, then there exists a dense subspace $\mathfrak{F} \subset \mathfrak{H}$ such that*

$$\int_\Delta (u(\varepsilon), c(\varepsilon, \varepsilon)v(\varepsilon)) \, \mathrm{d}\varepsilon = \lim_{\eta \downarrow 0} \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-\eta|t|} (\mathrm{e}^{\mathrm{i}tE} u, C\mathrm{e}^{\mathrm{i}tE} v) \, \mathrm{d}t,$$

for all $u, v \in \mathfrak{F}$.

Proof. Theorem 6.17 and its proof show that there exists a measurable set $\Delta_0 \subset \Delta$ such that $\Delta \setminus \Delta_0$ has Lebesgue measure zero and, for all $\varepsilon, \varepsilon' \in \Delta_0$,

$$c(\varepsilon', \varepsilon) = \sum_{n\in N} \kappa_n \, u_n^+(\varepsilon')(u_n^-(\varepsilon), \cdot)_{\mathfrak{h}_\varepsilon},$$

where N is a set which is at most countable, $\kappa_n > 0$, $\sum_{n\in N} \kappa_n = \|C\|_1$ and $(u_n^\pm)_{n\in N}$ are orthonormal families of $\mathfrak{H}$ such that

$$\sum_{n\in N} \kappa_n \|u_n^\pm(\varepsilon)\|^2_{\mathfrak{h}_\varepsilon} < \infty,$$

for all $\varepsilon \in \Delta_0$.

Let $u, v \in \mathfrak{H}$, for all $t \in \mathbb{R}$ we have

$$\begin{aligned}(\mathrm{e}^{\mathrm{i}tE}u, C\mathrm{e}^{\mathrm{i}tE}v) &= \int (u(\varepsilon'), c(\varepsilon',\varepsilon)v(\varepsilon))_{\mathfrak{h}_{\varepsilon'}}\, \mathrm{e}^{\mathrm{i}t(\varepsilon-\varepsilon')}\,\mathrm{d}\varepsilon\mathrm{d}\varepsilon' \\ &= \int \left(\sum_{n\in N}\kappa_n (u(\varepsilon'), u_n^+(\varepsilon'))_{\mathfrak{h}_{\varepsilon'}}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}\mathrm{e}^{\mathrm{i}t(\varepsilon-\varepsilon')}\right)\mathrm{d}\varepsilon\mathrm{d}\varepsilon'.\end{aligned}$$

Since $\|u_n^\pm\| = 1$, we have

$$\int |(u(\varepsilon'), u_n^+(\varepsilon'))_{\mathfrak{h}_{\varepsilon'}}\,(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_{k(\varepsilon)}}|\,\mathrm{d}\varepsilon\mathrm{d}\varepsilon' \le \|u\|\,\|v\|,$$

and thus

$$\sum_{n\in N}\kappa_n \int |(u(\varepsilon'), u_n^+(\varepsilon'))_{\mathfrak{h}_{\varepsilon'}}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}|\,\mathrm{d}\varepsilon\mathrm{d}\varepsilon' \le \sum_{n\in N}\kappa_n\|u\|\,\|v\| < \infty.$$

Fubini's theorem allows us to conclude that for $\eta > 0$,

$$\begin{aligned}&\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(\mathrm{e}^{\mathrm{i}tE}u, C\mathrm{e}^{\mathrm{i}tE}v)\,\mathrm{d}t \\ &= \sum_{n\in N}\kappa_n \int\left(\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u(\varepsilon'), u_n^+(\varepsilon'))_{\mathfrak{h}_{\varepsilon'}}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}\mathrm{e}^{\mathrm{i}t(\varepsilon-\varepsilon')}\,\mathrm{d}t\right)\mathrm{d}\varepsilon\mathrm{d}\varepsilon' \\ &= 2\pi\sum_{n\in N}\kappa_n\int (u(\varepsilon'), u_n^+(\varepsilon'))_{\mathfrak{h}_{\varepsilon'}}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}\,\delta_\eta(\varepsilon-\varepsilon')\,\mathrm{d}\varepsilon\mathrm{d}\varepsilon' \\ &= 2\pi\sum_{n\in N}\kappa_n\int \overline{F_n^+(\varepsilon)}(\delta_\eta \star F_n^-)(\varepsilon)\,\mathrm{d}\varepsilon, \end{aligned}\tag{160}$$

where $F_n^+(\varepsilon) = (u_n^+(\varepsilon), u(\varepsilon))_{\mathfrak{h}_\varepsilon}$, $F_n^-(\varepsilon) = (u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}$ and

$$\delta_\eta(\varepsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}t\varepsilon-\eta|t|}\,\mathrm{d}t = \frac{1}{\pi}\,\frac{\eta}{\varepsilon^2+\eta^2}.$$

Recall that the set $\mathfrak{F} \equiv \{u \in \mathfrak{H} \mid |||u||| \equiv \sup_{\varepsilon\in\Delta}\|u(\varepsilon)\|_{\mathfrak{h}_\varepsilon} < \infty\}$ is dense in $\mathfrak{H}$. For $u, v \in \mathfrak{F}$ the Cauchy-Schwarz inequality in $\mathfrak{h}_\varepsilon$ implies that $F_n^\pm \in L^2(\Delta, \mathrm{d}\varepsilon)$. Since $\mathrm{s}-\lim\limits_{\eta\downarrow 0}\delta_\eta\star = I$ in $L^2(\mathbb{R})$ we have

$$\lim_{\eta\downarrow 0}\int \overline{F_n^+(\varepsilon)}(\delta_\eta\star F_n^-)(\varepsilon)\,\mathrm{d}\varepsilon = \int\overline{F_n^+(\varepsilon)}F_n^-(\varepsilon)\,\mathrm{d}\varepsilon = \int (u(\varepsilon), u_n^+(\varepsilon))_{\mathfrak{h}_\varepsilon}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\varepsilon,$$

for all $n \in N$ and all $u, v \in \mathfrak{F}$. Since $\delta_\eta \in L^1(\mathbb{R})$ and $\|\delta_\eta\|_1 = \int\delta_\eta(\varepsilon)\,\mathrm{d}\varepsilon = 1$, the Cauchy-Schwarz and Young inequalities imply

$$\begin{aligned}&\left|\int\overline{F_n^+(\varepsilon)}(\delta_\eta\star F_n^-)(\varepsilon)\,\mathrm{d}\varepsilon\right| \le \left(\int|F_n^+(\varepsilon)|^2\,\mathrm{d}\varepsilon\right)^{1/2}\left(\int|F_n^-(\varepsilon)|^2\,\mathrm{d}\varepsilon\right)^{1/2} \\ &\le \left(\int\|u_n^+(\varepsilon)\|_{\mathfrak{h}_\varepsilon}^2\,\|u(\varepsilon)\|_{\mathfrak{h}_\varepsilon}^2\,\mathrm{d}\varepsilon\right)^{1/2}\left(\int\|u_n^-(\varepsilon)\|_{\mathfrak{h}_\varepsilon}^2\,\|v(\varepsilon)\|_{\mathfrak{h}_\varepsilon}^2\,\mathrm{d}\varepsilon\right)^{1/2} \\ &\le \left(|||u|||^2\int\|u_n^+(\varepsilon)\|_{\mathfrak{h}_\varepsilon}^2\,\mathrm{d}\varepsilon\right)^{1/2}\left(|||v|||^2\int\|u_n^-(\varepsilon)\|_{\mathfrak{h}_\varepsilon}^2\,\mathrm{d}\varepsilon\right)^{1/2} = |||u|||\,|||v|||,\end{aligned}$$

and the dominated convergence theorem applies to the right hand side of the identity (160)

$$\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty} \mathrm{e}^{-\eta|t|}(\mathrm{e}^{\mathrm{i}tE}u, C\mathrm{e}^{\mathrm{i}tE}v)\,\mathrm{d}t = 2\pi\sum_{n\in N}\kappa_n\int \overline{F_n^+(\varepsilon)}F_n^-(\varepsilon)\,\mathrm{d}\varepsilon$$
$$= 2\pi\sum_{n\in N}\kappa_n\int (u(\varepsilon), u_n^+(\varepsilon))_{\mathfrak{h}_\varepsilon}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\varepsilon.$$

Finally, Fubini's theorem allows us to conclude that

$$\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty} \mathrm{e}^{-\eta|t|}(\mathrm{e}^{\mathrm{i}tE}u, C\mathrm{e}^{-\mathrm{i}tE}v)\,\mathrm{d}t$$
$$= 2\pi\int\sum_{n\in N}\kappa_n(u(\varepsilon), u_n^+(\varepsilon))_{\mathfrak{h}_\varepsilon}(u_n^-(\varepsilon), v(\varepsilon))_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\varepsilon$$
$$= 2\pi\int (u(\varepsilon), c(\varepsilon,\varepsilon)v(\varepsilon))_{\mathfrak{h}_\varepsilon}\,\mathrm{d}\varepsilon,$$

for all $u, v\in\mathfrak{F}$. □

Remark 6.1 Theorem 6.17 and Lemmas 6.18 and 6.19 are generalized without difficulty to operators

$$C:\int^{\oplus}\mathfrak{h}_1(\varepsilon)\,\mathrm{d}\varepsilon\to\int^{\oplus}\mathfrak{h}_2(\varepsilon)\,\mathrm{d}\varepsilon,$$

it suffices in fact to identify them with operators

$$C':\int^{\oplus}\mathfrak{h}_1(\varepsilon)\oplus\mathfrak{h}_2(\varepsilon)\,\mathrm{d}\varepsilon\to\int^{\oplus}\mathfrak{h}_2(\varepsilon)\oplus\mathfrak{h}_2(\varepsilon)\,\mathrm{d}\varepsilon.$$

To apply the previous lemma to the calculation of the current, we shall use the following result.

Proposition 6.20 *Under Hypotheses(H1), (H2), and (H3), for all $u, v\in\widetilde{\mathcal{H}}_k$ we have*

$$\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u, \mathrm{e}^{\mathrm{i}t\widetilde{H}_k}\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')}\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v)\,\mathrm{d}t = \sigma\delta_{\sigma\sigma'}(g(\widetilde{H}_k)u, \widetilde{P}_k^{\sigma}\widetilde{Q}_k\widetilde{P}_k^{\sigma}g(\widetilde{H}_k)v).$$

Proof. By remarking that

$$(u, \mathrm{e}^{\mathrm{i}t\widetilde{H}_k}\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')}\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v) = \frac{\mathrm{d}}{\mathrm{d}t}G^{(\sigma,\sigma')}(t),$$

with

$$G^{(\sigma,\sigma')}(t) = (h_\sigma^{(a)}(\widetilde{A}_k)\mathrm{e}^{\mathrm{i}t\widetilde{H}_k}g(\widetilde{H}_k)u, M_k^*QM_kh_{\sigma'}^{(a)}(\widetilde{A}_k)\mathrm{e}^{\mathrm{i}t\widetilde{H}_k}g(\widetilde{H}_k)v),$$

we obtain, after an integration by parts,

$$\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u, \mathrm{e}^{\mathrm{i}t\widetilde{H}_k}\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')}\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v)\,\mathrm{d}t = \eta\int_0^{\infty}\mathrm{e}^{-\eta t}(G^{(\sigma,\sigma')}(t) - G^{(\sigma,\sigma')}(-t))\,\mathrm{d}t,$$

and consequently

$$\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}(u,\mathrm{e}^{\mathrm{i}t\widetilde{H}_k}\widetilde{\Psi}^{\#(a,\sigma,\sigma')}_{Q,g,k}\mathrm{e}^{-\mathrm{i}t\widetilde{H}_k}v)\,\mathrm{d}t$$
$$=\mathrm{Abel}-\lim_{t\to\infty}G^{(\sigma,\sigma')}(t)-\mathrm{Abel}-\lim_{t\to-\infty}G^{(\sigma,\sigma')}(t).$$

To evaluate these Abelian limits, we invoke the propagation estimates. For $t>0$, we have

$$\begin{aligned}\|h_\sigma^{(a)}(\widetilde{A}_k)\mathrm{e}^{\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u\| &\le \|F(\sigma\widetilde{A}_k\ge a-1)\mathrm{e}^{\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u\|\\ &\le \|F(\sigma\widetilde{A}_k\ge a-1)\mathrm{e}^{\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)F(\sigma\widetilde{A}_k>\vartheta t)u\|\\ &+\|F(\sigma\widetilde{A}_k\ge a-1)\mathrm{e}^{\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)F(\sigma\widetilde{A}_k\le\vartheta t)u\|\\ &\le \|F(\sigma\widetilde{A}_k>\vartheta t)u\|\\ &+\|F((-\sigma)\widetilde{A}_k\le 1-a)\mathrm{e}^{-\mathrm{i}(-\sigma)t\widetilde{H}_k}g(\widetilde{H}_k)F((-\sigma)\widetilde{A}_k\ge-\vartheta t)u\|.\end{aligned}$$

When $t\to+\infty$ the first term on the right hand side of this inequality tends clearly to 0 for all $\vartheta>0$. By applying Proposition 4.27 to the second term it is possible to choose $\vartheta>0$ such that

$$\|F((-\sigma)\widetilde{A}_k\le 1-a)\mathrm{e}^{-\mathrm{i}(-\sigma)t\widetilde{H}_k}g(\widetilde{H}_k)F((-\sigma)\widetilde{A}_k\ge-\vartheta t)u\|\le c\,\langle a-1+\vartheta t\rangle^{-s},$$

for constants c and $s>0$. We thus have

$$\lim_{t\to+\infty}\|h_\sigma^{(a)}(\widetilde{A}_k)\mathrm{e}^{\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u\|=0,$$

and it follows that

$$\mathrm{Abel}-\lim_{t\to+\infty}G^{(\sigma,\sigma')}(t)=\lim_{t\to+\infty}G^{(\sigma,\sigma')}(t)=0,$$

if $\langle\sigma,\sigma'\rangle\neq\langle+,+\rangle$ and that

$$\mathrm{Abel}-\lim_{t\to-\infty}G^{(\sigma,\sigma')}(t)=\lim_{t\to-\infty}G^{(\sigma,\sigma')}(t)=0,$$

if $\langle\sigma,\sigma'\rangle\neq\langle-,-\rangle$. It remains to consider $G^{(\sigma,\sigma)}(\sigma t)$ for $t\to+\infty$. By writing

$$\begin{aligned}G^{(\sigma,\sigma)}(\sigma t)&=(h_\sigma^{(a)}(\widetilde{A}_k)\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u,M_k^*QM_kh_\sigma^{(a)}(\widetilde{A}_k)\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)v)\\ &=(\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u,M_k^*QM_k\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)v)\\ &-(\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u,M_k^*QM_k(1-h_\sigma^{(a)}(\widetilde{A}_k))\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)v)\\ &-((1-h_\sigma^{(a)}(\widetilde{A}_k))\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u,M_k^*QM_k\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)v)\\ &+((1-h_\sigma^{(a)}(\widetilde{A}_k))\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u,M_k^*QM_k(1-h_\sigma^{(a)}(\widetilde{A}_k))\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)v),\end{aligned}\tag{161}$$

we remark that

$$\begin{aligned}\|(1-h_\sigma^{(a)}(\widetilde{A}_k))\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u\|&\le\|F(\sigma\widetilde{A}_k\le a+1)\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)u\|\\ &\le\|F(\sigma\widetilde{A}_k\le a+1)\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)F(\sigma\widetilde{A}_k<a+1-\vartheta t)u\|\\ &+\|F(\sigma\widetilde{A}_k\le a+1)\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k}g(\widetilde{H}_k)F(\sigma\widetilde{A}_k\ge a+1-\vartheta t)u\|,\end{aligned}$$

and we conclude as before that

$$\lim_{t\to+\infty} \|(1-h_\sigma^{(a)}(\widetilde{A}_k))\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k} g(\widetilde{H}_k)u\| = 0,$$

which shows that the three last terms of the right hand side of the identity (161) vanish in this limit. The first term in turn is calculated as follows, by using the fact that Q commutes with H and the identity (137),

$$\begin{aligned}
&\lim_{t\to+\infty} (\mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k} g(\widetilde{H}_k)u, M_k^* Q M_k \mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k} g(\widetilde{H}_k)v) \\
&\quad = \lim_{t\to+\infty} (g(\widetilde{H}_k)u, \mathrm{e}^{\mathrm{i}\sigma t\widetilde{H}_k} M_k^* \mathrm{e}^{-\mathrm{i}\sigma tH} Q \mathrm{e}^{\mathrm{i}\sigma tH} M_k \mathrm{e}^{-\mathrm{i}\sigma t\widetilde{H}_k} g(\widetilde{H}_k)v) \\
&\quad = (g(\widetilde{H}_k)u, \Omega_k^{\sigma*} Q \Omega_k^\sigma g(\widetilde{H}_k)v) \\
&\quad = (g(\widetilde{H}_k)u, \widetilde{P}_k^\sigma \widetilde{Q}_k \widetilde{P}_k^\sigma g(\widetilde{H}_k)v).
\end{aligned}$$

□

6.6.5 Proof of Theorem 6.16

(i) We note that since $g \in C_0^\infty(\mathbb{R}\setminus\Sigma_H) \subset C_0^\infty(\mathbb{R}\setminus\Sigma_k)$, the spectrum of $\widetilde{H}_k$ is purely absolutely continuous on $\operatorname{supp} g$ by Corollary 5.3. We thus have $\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} = P_{\mathrm{ac}}(\widetilde{H}_k)\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')} P_{\mathrm{ac}}(\widetilde{H}_k)$.

(ii) The existence of the integral kernel $\psi_{Q,g,k}^{\#(a,\sigma,\sigma')}$ is a direct consequence of the fact that $\widetilde{\Psi}_{Q,g,k}^{\#(a,\sigma,\sigma')}$ is trace-class and of Theorem 6.17.

(iii) Lemma 6.19 and Proposition 6.20 give us

$$\begin{aligned}
\int (u(\varepsilon), \psi_{Q,g,k}^{\#(a,\sigma,\sigma')}(\varepsilon,\varepsilon)v(\varepsilon))_{\mathfrak{h}_k(\varepsilon)}\,\mathrm{d}\varepsilon &= \frac{1}{2\pi}\sigma\delta_{\sigma\sigma'}(g(\widetilde{H}_k)u, \widetilde{P}_k^\sigma \widetilde{Q}_k \widetilde{P}_k^\sigma g(\widetilde{H}_k)v) \\
&= \frac{1}{2\pi}\sigma\delta_{\sigma\sigma'} \int (u(\varepsilon), g(\varepsilon)p_k^\sigma(\varepsilon)q_k(\varepsilon)p_k^\sigma(\varepsilon)g(\varepsilon)v(\varepsilon))_{\mathfrak{h}_k(\varepsilon)}\,\mathrm{d}\varepsilon,
\end{aligned}$$

for all $u, v \in \mathfrak{F}_k$, a dense subspace of $\widetilde{\mathcal{H}}_{k,\mathrm{ac}}$. Lemma 6.18 allows us to conclude that

$$\psi_{Q,g,k}^{\#(a,\sigma,\sigma')}(\varepsilon,\varepsilon) = \frac{\sigma}{2\pi}\delta_{\sigma\sigma'} g(\varepsilon)p_k^\sigma(\varepsilon)q_k(\varepsilon)p_k^\sigma(\varepsilon)g(\varepsilon),$$

for almost all $\varepsilon \in \mathbb{R}$. □

6.7 The Landauer-Büttiker formula

We are now prepared to prove Theorem 6.7.

Starting from (158) we obtain the following representation of the steady current

$$\begin{aligned}
\operatorname{tr}(\Omega_j^- \widetilde{T}_j \Omega_j^{-*} \Psi_{Q,g,k}^{(a)}) = \int \operatorname{tr}_{\mathfrak{h}_j(\varepsilon)} \Big(t_j(\varepsilon) \Big\{ s_{jk}^*(\varepsilon)\psi_{Q,g,k}^{\#(a,+,+)}(\varepsilon,\varepsilon)s_{kj}(\varepsilon) \\
+ \delta_{jk}\Big(s_{kk}^*(\varepsilon)\psi_{Q,g,k}^{\#(a,+,-)}(\varepsilon,\varepsilon)p_k^-(\varepsilon) + p_k^-(\varepsilon)\psi_{Q,g,k}^{\#(a,-,+)}(\varepsilon,\varepsilon)s_{kk}(\varepsilon) + p_k^-(\varepsilon)\psi_{Q,g,k}^{\#(a,-,-)}(\varepsilon,\varepsilon)p_k^-(\varepsilon)\Big)\Big\}\Big)\,\mathrm{d}\varepsilon.
\end{aligned}$$

By inserting Expression (159) we find

$$\operatorname{tr}(\Omega_j^- \widetilde{T}_j \Omega_j^{-*} \Psi_{Q,g,k}^{(a)}) = \int g(\varepsilon)^2 \operatorname{tr}_{\mathfrak{h}_j(\varepsilon)} \left(t_j(\varepsilon) \left\{ s_{jk}^*(\varepsilon) q_k^+(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} q_j^-(\varepsilon) \right\} \right) \frac{\mathrm{d}\varepsilon}{2\pi},$$

where $q_k^\pm(\varepsilon) \equiv p_k^\pm(\varepsilon) q_k(\varepsilon) p_k^\pm(\varepsilon)$.

To control the limit (143) and thus obtain the steady current of an eventually unbounded charge we shall use the following result, adapted from Theorem 6 of Section 7.6 in [Y] to our situation.

Lemma 6.21 *Under Hypotheses (H1), (H2), (H3), and (H5), $s_{jk}(\varepsilon) - \delta_{jk} p_k^\pm(\varepsilon)$ is trace-class for almost all $\varepsilon \in \mathbb{R}$. Furthermore, there exists a constant c such that, for any measurable bounded function $f : \mathbb{R} \to \mathbb{R}$ and any interval $\Delta \subset \mathbb{R}$*

$$\int_\Delta f(\varepsilon)^2 \, \| s_{jk}(\varepsilon) - \delta_{jk} p_k^\pm(\varepsilon) \|_1 \, \mathrm{d}\varepsilon \le c \left(\operatorname{ess-supp}_{\varepsilon \in \Delta} \langle \varepsilon \rangle^{\nu+1} |f(\varepsilon)| \right)^2 .$$

Proof. Without loss of generality we may suppose that $f \geq 0$. Let $K \subset \Delta$ be compact, set $g \equiv f 1_K$ and note that

$$(g(\widetilde{H}_j)u, (S_{jk} - \delta_{jk} \widetilde{P}_k^+) g(\widetilde{H}_k) v) = -(\Omega_j^+ g(\widetilde{H}_j) u, (\Omega_k^+ - \Omega_k^-) g(\widetilde{H}_k) v), \tag{162}$$

$$(g(\widetilde{H}_j)u, (S_{jk} - \delta_{jk} \widetilde{P}_k^-) g(\widetilde{H}_k) v) = -((\Omega_j^+ - \Omega_j^-) g(\widetilde{H}_j) u, \Omega_k^- g(\widetilde{H}_k) v). \tag{163}$$

For all $u \in \widetilde{\mathscr{H}}_{j,\mathrm{ac}}$, $v \in \widetilde{\mathscr{H}}_{k,\mathrm{ac}}$, Relation (162) yields, after passing to the Abelian limit and integrating by parts,

$$\begin{aligned}
(g(\widetilde{H}_j)u, (S_{jk} - \delta_{jk}\widetilde{P}_k^+) g(\widetilde{H}_k) v) &= -\lim_{t\to\infty} (\Omega_j^+ g(\widetilde{H}_j) u, (\mathrm{e}^{\mathrm{i}tH} M_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} - \mathrm{e}^{-\mathrm{i}tH} M_k \mathrm{e}^{\mathrm{i}t\widetilde{H}_k}) g(\widetilde{H}_k) v) \\
&= -\lim_{\eta\downarrow 0} \eta \int_0^\infty \mathrm{e}^{-\eta t} (\Omega_j^+ g(\widetilde{H}_j) u, (\mathrm{e}^{\mathrm{i}tH} M_k \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} - \mathrm{e}^{-\mathrm{i}tH} M_k \mathrm{e}^{\mathrm{i}t\widetilde{H}_k}) g(\widetilde{H}_k) v) \, \mathrm{d}t \\
&= -\lim_{\eta\downarrow 0} \int_{-\infty}^\infty \mathrm{e}^{-\eta|t|} (\Omega_j^+ g(\widetilde{H}_j) u, \mathrm{e}^{\mathrm{i}tH} \mathrm{i}(H M_k - M_k \widetilde{H}_k) \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} g(\widetilde{H}_k) v) \, \mathrm{d}t.
\end{aligned}$$

By using the intertwining relations of the Møller operators we obtain

$$(g(\widetilde{H}_j)u, (S_{jk} - \delta_{jk}\widetilde{P}_k^+) g(\widetilde{H}_k) v) = \lim_{\eta\downarrow 0} \int_{-\infty}^\infty \mathrm{e}^{-\eta|t|} (\mathrm{e}^{-\mathrm{i}t\widetilde{H}_j} u, C \mathrm{e}^{-\mathrm{i}t\widetilde{H}_k} v) \, \mathrm{d}t,$$

where

$$C \equiv -\mathrm{i}\Omega_j^{+*} g(H)(HM_k - M_k \widetilde{H}_k) g(\widetilde{H}_k).$$

The identity

$$\begin{aligned}
g(H)(HM_k - M_k\widetilde{H}_k) g(\widetilde{H}_k) = {} & g_1(H) \left((H+\mathrm{i})^{-\nu} M_k - M_k (\widetilde{H}_k + \mathrm{i})^{-\nu} \right) g(\widetilde{H}_k) \\
& - g_1(H) \left((H+\mathrm{i})^{-\nu-1} M_k - M_k (\widetilde{H}_k + \mathrm{i})^{-\nu-1} \right) (\widetilde{H}_k + \mathrm{i}) g(\widetilde{H}_k),
\end{aligned}$$

where $g_1(x) = g(x)(x+\mathrm{i})^{\nu+1}$, and Lemma 6.1 allow us to conclude that C is trace-class. Furthermore, since $\|\Omega_j^{+*}\| \le 1$, we have the estimate

$$\begin{aligned}\|C\|_1 \le \|g_1(H)\|\,\|(H+\mathrm{i})^{-\nu}M_k - M_k(\widetilde{H}_k+\mathrm{i})^{-\nu}\|_1\|g(\widetilde{H}_k)\| \\ + \|g_1(H)\|\,\|(H+\mathrm{i})^{-\nu-1}M_k - M_k(\widetilde{H}_k+\mathrm{i})^{-\nu-1}\|_1\,\|(\widetilde{H}_k+\mathrm{i})g(\widetilde{H}_k)\|,\end{aligned}$$

and it follows that there exists a constant c_1 such that

$$\|C\|_1 \le c_1 \left(\underset{\varepsilon\in\Delta}{\mathrm{ess}-\mathrm{supp}}\, \langle\varepsilon\rangle^{\nu+1} f(\varepsilon)\right)^2. \tag{164}$$

By Lemma 6.17, C has an integral kernel $c(\varepsilon',\varepsilon)$ and Lemma 6.19 allows us to write

$$\frac{1}{2\pi}\int g(\varepsilon)^2 (u(\varepsilon), (s_{jk}(\varepsilon)-\delta_{jk}p_k^+(\varepsilon))v(\varepsilon))_{\mathfrak{h}_j(\varepsilon)}\mathrm{d}\varepsilon = \int (u(\varepsilon), c(\varepsilon,\varepsilon)v(\varepsilon))_{\mathfrak{h}_j(\varepsilon)}\mathrm{d}\varepsilon,$$

for $u\in\mathfrak{F}_j$ and $v\in\mathfrak{F}_k$, $\mathfrak{F}_j$, $\mathfrak{F}_k$ being dense subspaces of $\widetilde{\mathscr{H}}_{j,\mathrm{ac}}$ and $\widetilde{\mathscr{H}}_{k,\mathrm{ac}}$. By Lemma 6.18 we have

$$\frac{1}{2\pi} g(\varepsilon)^2 \left(s_{jk}(\varepsilon) - \delta_{jk}p_k^\pm(\varepsilon)\right) = c(\varepsilon,\varepsilon),$$

for almost every $\varepsilon\in\mathbb{R}$, and invoking Lemma 6.17 we obtain

$$\begin{aligned}\int_K f(\varepsilon)^2\,\|s_{jk}(\varepsilon)-\delta_{jk}p_k^+(\varepsilon)\|_1\,\mathrm{d}\varepsilon &\le \int g(\varepsilon)^2\|s_{jk}(\varepsilon)-\delta_{jk}p_k^+(\varepsilon)\|_1\,\mathrm{d}\varepsilon \\ &\le 2\pi\,\|C\|_1 \\ &\le c_2\left(\underset{\varepsilon\in\Delta}{\mathrm{ess}-\mathrm{supp}}\,\langle\varepsilon\rangle^{\nu+1}f(\varepsilon)\right)^2,\end{aligned}$$

and thus

$$\begin{aligned}\int_\Delta f(\varepsilon)^2\,\|s_{jk}(\varepsilon)-\delta_{jk}p_k^+(\varepsilon)\|_1\,\mathrm{d}\varepsilon &= \sup_{\substack{K\subset\Delta\\ K\text{ compact}}} \int_K f(\varepsilon)^2\,\|s_{jk}(\varepsilon)-\delta_{jk}p_k^+(\varepsilon)\|_1\,\mathrm{d}\varepsilon \\ &\le c_2\left(\underset{\varepsilon\in\Delta}{\mathrm{ess}-\mathrm{supp}}\,\langle\varepsilon\rangle^{\nu+1}f(\varepsilon)\right)^2.\end{aligned}$$

The case where p_k^+ is replaced by p_k^- can be handled in a similar way, starting from Eq. (163).
□

Let Q be a temperate charge such that $\mathrm{Dom}(H^\alpha)\subset\mathrm{Dom}(Q)$ for some $\alpha\ge 0$. Then $Q(H+\mathrm{i})^{-\alpha}$ is bounded and it follows from the identity (137) that $\widetilde{P}_k^\pm\widetilde{Q}_k(\widetilde{H}_k+\mathrm{i})^{-\alpha}\widetilde{P}_k^\pm$ is bounded. We thus have

$$c_1 \equiv \max_{k\in\{1,\dots,M\}} \underset{\varepsilon\in\mathbb{R}}{\mathrm{ess}-\mathrm{supp}}\,\langle\varepsilon\rangle^{-\alpha}\|q_k^\pm(\varepsilon)\|_{\mathfrak{h}_k(\varepsilon)} < \infty.$$

We shall denote by $q_{\epsilon,k}(\varepsilon) = (1+\epsilon\varepsilon^2)^{-\alpha/2} q_k(\varepsilon)$ the fibers of the regularized charge $\widetilde{Q}_{\epsilon,k} = \widetilde{Q}_k(I+\epsilon\widetilde{H}_k^2)^{-\alpha}$. Similarly, if for $j \in \{1,\dots,M\}$, $\widetilde{T}_j$ denotes the generator of a τ_j-invariant, gauge invariant, quasi-free state on $\mathcal{O}_j$ such that $\operatorname{Ran}(\widetilde{T}_j) \subset \operatorname{Dom}(\widetilde{H}_j^{\alpha+\nu+1})$ then $\widetilde{H}_j^{\alpha+\nu+1}\widetilde{T}_j$ is bounded and

$$c_2 \equiv \max_{j\in\{1,\dots,M\}} \operatorname*{ess-supp}_{\varepsilon\in\mathbb{R}} \langle\varepsilon\rangle^{\alpha+\nu+1} \|t_j(\varepsilon)\| < \infty.$$

Since $s_{jk}^*(\varepsilon) = s_{kj}(\varepsilon)^*$ we have

$$0 \le s_{jk}^*(\varepsilon) s_{kj}(\varepsilon) \le \sum_{l=1}^M s_{jl}^*(\varepsilon) s_{lj}(\varepsilon) = p_j^-(\varepsilon) \le I,$$

and consequently, $\|s_{kj}(\varepsilon)\| \le \|p_j^-(\varepsilon)\| \le 1$. Charge conservation, Eq. (139), thus writes

$$q_j^-(\varepsilon) = \sum_{l=1}^M s_{jl}^*(\varepsilon) q_l^+(\varepsilon) s_{lj}(\varepsilon),$$

from which we obtain the identity

$$s_{jk}^*(\varepsilon) q_k^+(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} q_j^-(\varepsilon) = \sum_{l=1}^M (\delta_{kl} - \delta_{kj}) s_{jl}^*(\varepsilon) q_l^+(\varepsilon)(s_{lj}(\varepsilon) - \delta_{lj} p_j^-(\varepsilon)),$$

and then the inequality

$$\|s_{jk}^*(\varepsilon) q_k^+(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} q_j^-(\varepsilon)\|_1 \le \sum_{l=1}^M \|q_l^+(\varepsilon)\| \, \|s_{lj}(\varepsilon) - \delta_{lj} p_j^-(\varepsilon)\|_1.$$

We thus have

$$\begin{aligned}\sum_{j=1}^M \left| \operatorname{tr}_{\mathfrak{h}_j(\varepsilon)} \left(t_j(\varepsilon) \left\{ s_{jk}^*(\varepsilon) q_{\epsilon,k}^+(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} q_{\epsilon,j}^-(\varepsilon) \right\} \right) \right| &\le \sum_{j,l=1}^M \|t_j(\varepsilon)\| \, \|q_l^+(\varepsilon)\| \, \|s_{lj}(\varepsilon) - \delta_{lj} p_j^-(\varepsilon)\|_1 \\ &\le c_1 c_2 \langle\varepsilon\rangle^{-\nu-1} \sum_{j,l=1}^M \|s_{lj}(\varepsilon) - \delta_{lj} p_j^-(\varepsilon)\|_1,\end{aligned}$$

and Lemma 6.21 allows us to conclude that the left hand side of this inequality belongs to $L^1(\mathbb{R}, \mathrm{d}\varepsilon)$. By the dominated convergence theorem, we conclude that for all $g \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$ such that $0 \le g \le 1$

$$\lim_{\epsilon\downarrow 0} \sum_{j=1}^M \operatorname{tr}(\Omega_j^- \widetilde{T}_j \Omega_j^{-*} \Psi_{Q_\epsilon,g,k}^{(a)}) = \int g(\varepsilon)^2 \operatorname{tr}_{\mathfrak{h}_j(\varepsilon)} \left(t_j(\varepsilon) \left\{ s_{jk}^*(\varepsilon) q_k^+(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} q_j^-(\varepsilon) \right\} \right) \frac{\mathrm{d}\varepsilon}{2\pi}.$$

Similarly, if $g_n \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$ is a sequence such that $0 \le g_n \le 1$ and $\lim_n g_n(x) = 1$ for almost all $x \in \mathbb{R}$ we have

$$\lim_n \sum_{j=1}^M \operatorname{tr}(\Omega_j^- \widetilde{T}_j \Omega_j^{-*} \Psi_{Q,g_n,k}^{(a)}) = \int \operatorname{tr}_{\mathfrak{h}_j(\varepsilon)} \left(t_j(\varepsilon) \left\{ s_{jk}^*(\varepsilon) q_k^+(\varepsilon) s_{kj}(\varepsilon) - \delta_{kj} q_j^-(\varepsilon) \right\} \right) \frac{\mathrm{d}\varepsilon}{2\pi},$$

which concludes the proof of Theorem 6.7.

A Proof of Lemma 6.1

We begin by proving two auxiliary lemmas based on Hypothesis (H5).

Lemma A.1 *Under Hypothesis (H5) we have*

$$\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k) \in \mathscr{B}(\widetilde{\mathscr{H}}^{s+j/2}_k, \widetilde{\mathscr{H}}^s_k),$$

for $1 \le j \le s + j \le 4\nu$, $k \in \{1, \dots, M\}$ *and* $r \ge 0$. *Furthermore, if* s *is an integer then the formula*

$$(\widetilde{H}_k - z)^s \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k) = \sum_{l=0}^{s} \binom{s}{l} (-\mathrm{i})^l \mathrm{ad}^{j+l}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{s-l}, \tag{165}$$

holds on $\widetilde{\mathscr{H}}^{s+j/2}_k$.

Proof. By hypothesis the assertion is verified for $s = 0$. By interpolation, it suffice to prove the assertion for integer s. We begin by remarking that the identity (81) implies that for all $z \in \mathrm{Res}(\widetilde{H}_k)$

$$(\widetilde{H}_k - z)^{-s-j/2} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k) = \sum_{l=0}^{s} \binom{s}{l} \mathrm{i}^l (\widetilde{H}_k - z)^{-l-j/2} \mathrm{ad}^{j+l}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-s}.$$

This formula is purely algebraic. However, it is justified by Hypothesis (H5) (i) which implies, by duality, that $\mathrm{ad}^{j+l}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k) \in \mathscr{B}(\widetilde{\mathscr{H}}_k, \widetilde{\mathscr{H}}^{-(j+l)/2}_k)$ for $1 \le l + j \le 4\nu$. For $l \in \{0, \dots, n\}$ the estimate

$$\begin{aligned}
&\|(\widetilde{H}_k - z)^{-l-j/2} \mathrm{ad}^{j+l}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-s}\|_{\mathscr{B}(\widetilde{\mathscr{H}}^{-s}_k, \widetilde{\mathscr{H}}_k)} \\
&\quad \le \|(\widetilde{H}_k - z)^{-l-j/2}\|_{\mathscr{B}(\widetilde{\mathscr{H}}^{-(j+l)/2}_k, \widetilde{\mathscr{H}}^{l/2}_k)} \|\mathrm{ad}^{j+l}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)\|_{\mathscr{B}(\widetilde{\mathscr{H}}_k, \widetilde{\mathscr{H}}^{-(j+l)/2}_k)} \|(\widetilde{H}_k - z)^{-s}\|_{\mathscr{B}(\widetilde{\mathscr{H}}^{-s}_k, \widetilde{\mathscr{H}}_k)},
\end{aligned}$$

shows that $(\widetilde{H}_k - z)^{-s-j/2} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)$ is bounded from $\widetilde{\mathscr{H}}^{-s}_k$ into $\widetilde{\mathscr{H}}_k$. We conclude that, for $s + j \le 4\nu$ we have $\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k) \in \mathscr{B}(\widetilde{\mathscr{H}}^{-s}_k, \widetilde{\mathscr{H}}^{-s-j/2}_k)$ and the assertion follows by duality. By taking the adjoint of the identity (81) we obtain

$$\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-s-j/2} = \sum_{l=0}^{s} \binom{s}{l} (-\mathrm{i})^l (\widetilde{H}_k - z)^{-s} \mathrm{ad}^{j+l}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-l-j/2},$$

which shows that (165) holds. □

Lemma A.2 *Under Hypotheses (H1), (H2), and (H5) we have*

$$\begin{aligned}
(H - z)^{-1} M^{(r)}_k - M^{(r)}_k (\widetilde{H}_k - z)^{-1} &= \sum_{j=1}^{l-1} \mathrm{i}^j J^{(r)}_k \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-(j+1)} \\
&\quad + \mathrm{i}^l (H - z)^{-1} J^{(r)}_k \mathrm{ad}^l_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-l},
\end{aligned}$$

for all $z \in \mathrm{Res}(H) \cap \mathrm{Res}(\widetilde{H}_k)$, $k \in \{1, \dots, M\}$, $r \ge 0$ *and* $l \le 2\nu$.

Proof. Lemma A.1 allows us to write, for $j = 1,\dots,2\nu$ and for all $u \in \widetilde{\mathcal{H}}_k^{1+j/2}$, by invoking Hypothesis (H1) (vi) then the identity (107) and then Hypothesis (H5) (ii)

$$\begin{aligned} v \equiv J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u &= J_k^{(r-1)} \tilde{1}_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= J_k^{(r-1)} \widetilde{\chi}_k^{(r-1)} \tilde{1}_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= J_k^{(r-1)} \widetilde{\chi}_k^{(r-1)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u. \end{aligned}$$

Hypothesis (H2) (ii) implies $v \in \mathrm{Dom}(H)$ and $Hv = J_k^{(r-1)} \widetilde{H}_k \widetilde{\chi}_k^{(r-1)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u$. By using Hypothesis (H5) (ii) and the identity (107) we may continue with

$$\begin{aligned} Hv &= J_k^{(r-1)} \widetilde{H}_k \widetilde{\chi}_k^{(r-1)} \tilde{1}_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= J_k^{(r-1)} \widetilde{H}_k \tilde{1}_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= J_k^{(r-1)} \widetilde{H}_k \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u. \end{aligned}$$

In a similar manner, we show that

$$J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{H}_k u = J_k^{(r-1)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{H}_k u,$$

and we obtain

$$\begin{aligned} J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{H}_k u - H J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u &= -J_k^{(r-1)} [\widetilde{H}_k, \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})]u \\ &= \mathrm{i} J_k^{(r-1)} \mathrm{ad}^{j+1}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= \mathrm{i} J_k^{(r-1)} \tilde{1}_k^{(r)} \mathrm{ad}^{j+1}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= \mathrm{i} J_k^{(r)} \tilde{1}_k^{(r)} \mathrm{ad}^{j+1}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u \\ &= \mathrm{i} J_k^{(r)} \mathrm{ad}^{j+1}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u. \end{aligned}$$

By setting $R \equiv (H - z)^{-1}$ and $\widetilde{R} = (\widetilde{H}_k - z)^{-1}$, this identity allows us to write, for all $u \in \widetilde{\mathcal{H}}_k^{j/2}$,

$$\begin{aligned} R J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})u - J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R} u &= R(J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{H}_k - H J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})) \widetilde{R} u \\ &= \mathrm{i} R J_k^{(r)} \mathrm{ad}^{j+1}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R} u. \end{aligned}$$

We thus obtain the formula

$$R J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R}^j = J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R}^{j+1} + \mathrm{i} R J_k^{(r)} \mathrm{ad}^{j+1}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R}^{j+1},$$

and by iteration,

$$\mathrm{i} R J_k^{(r)} \mathrm{ad}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R} = \sum_{j=1}^{l-1} \mathrm{i}^j J_k^{(r)} \mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R}^{j+1} + \mathrm{i}^l R J_k^{(r)} \mathrm{ad}^l_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) \widetilde{R}^l.$$

We conclude by remarking that

$$RM_k^{(r)} - M_k^{(r)}\widetilde{R} = \mathrm{i}RJ_k^{(r)}\mathrm{ad}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})\widetilde{R},$$

c.f. Lemma 5.4. □

Proof of Lemma 6.1. By differentiation of the formula in Lemma A.2 with $l = 2\nu$ we obtain

$$\begin{aligned}(H-z)^{-\ell}M_k^{(r)} - M_k^{(r)}(\widetilde{H}_k - z)^{-\ell} &= \sum_{j=1}^{2\nu-1} \mathrm{i}^j J_k^{(r)}\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-\ell-j} \\ &+ \mathrm{i}^{2\nu}\sum_{j=0}^{\ell-1}\binom{\ell-1}{j}(H-z)^{-\ell+j}J_k^{(r)}\mathrm{ad}^{2\nu}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-2\nu-j}.\end{aligned}$$

Thus, it suffices to show that each factor of the type $\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-q}$ appearing on the right hand side of this relation is trace-class. We note that for each one of these factors we have $p \le 2\nu$ and $q \ge \nu + p/2$.
For all $p \le 2\nu$, Hypotheses (H1) (ii) and (H5) (ii) imply that $(I - \widetilde{\chi}_k^{(r-1)})\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) = 0$. By (H5) (iii) we also have $\widetilde{\chi}_k^{(r+1)}\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) = 0$. Consequently, we have

$$\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}) = \varphi_k^{(r)}\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)}), \tag{166}$$

where $\varphi_k^{(r)} \equiv (\widetilde{\chi}_k^{(r-1)} - \widetilde{\chi}_k^{(r+1)})$. By writing

$$\begin{aligned}\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-q} &= \varphi_k^{(r)}\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-q} \\ &= \left(\varphi_k^{(r)}(\widetilde{H}_k + \mathrm{i})^{-\nu}\right)\left((\widetilde{H}_k + \mathrm{i})^{\nu}\mathrm{ad}^p_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-q}\right),\end{aligned}$$

we remark that the first factor of the right hand side is trace-class by Hypothesis (H5) (iv) while the second factor is bounded by Lemma A.1 as soon as $q \ge \nu + p/2$.
Lemma A.2 and the Helffer-Sjöstrand formula (6) allow us to write

$$f(H)M_k^{(r)} - M_k^{(r)}f(\widetilde{H}_k) = \sum_{j=1}^{2\nu-1}\frac{\mathrm{i}^j}{j!}J_k^{(r)}\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})f^{(j)}(\widetilde{H}_k) + \mathscr{R},$$

where the remainder is given by

$$\mathscr{R} = \frac{\mathrm{i}^{2\nu-1}}{2\pi}\int \bar{\partial}\tilde{f}(z)(H-z)^{-1}J_k^{(r)}\mathrm{ad}^{2\nu}_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})(\widetilde{H}_k - z)^{-2\nu}\,\mathrm{d}z \wedge \mathrm{d}\bar{z},$$

and where $\tilde{f}$ is an almost-analytic extension of f of order $2\nu + 1$. By writing

$$\begin{aligned}\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})f^{(j)}(\widetilde{H}_k) &= \varphi_k^{(r)}\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})f^{(j)}(\widetilde{H}_k) \\ &= \left(\varphi_k^{(r)}(\widetilde{H}_k + \mathrm{i})^{-\nu}\right)\left((\widetilde{H}_k + \mathrm{i})^{\nu}\mathrm{ad}^j_{\widetilde{H}_k}(\widetilde{\chi}_k^{(r)})f^{(j)}(\widetilde{H}_k)\right),\end{aligned}$$

we note as before that the first factor of the right hand side is trace-class and the second factor is bounded.

The remainder $\mathscr{R}$ is treated in a similar manner with

$$\mathrm{ad}^{2\nu}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-2\nu} = \left(\varphi^{(r)}_k(\widetilde{H}_k + \mathrm{i})^{-\nu}\right)\left((\widetilde{H}_k + \mathrm{i})^{\nu}\mathrm{ad}^{2\nu}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-2\nu}\right),$$

where the first factor of the right hand side is trace-class. Writing the second factor as

$$(\widetilde{H}_k + \mathrm{i})^{\nu}\mathrm{ad}^{2\nu}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k - z)^{-2\nu} = \left((\widetilde{H}_k + \mathrm{i})^{\nu}\mathrm{ad}^{2\nu}_{\widetilde{H}_k}(\widetilde{\chi}^{(r)}_k)(\widetilde{H}_k + \mathrm{i})^{-2\nu}\right)\left((\widetilde{H}_k + \mathrm{i})^{2\nu}(\widetilde{H}_k - z)^{-2\nu}\right),$$

we observe that the first factor of the right hand side is bounded by Lemma A.1. The second factor is bounded by

$$\|(\widetilde{H}_k + \mathrm{i})^{2\nu}(\widetilde{H}_k - z)^{-2\nu}\| \le c|\mathrm{Im} z|^{-2\nu},$$

for $z \in \mathrm{supp}\,\tilde{f}$. We deduce that $\mathscr{R}$ is trace-class. □

B Proof of Lemma 6.12

In this appendix we prove the trace-norm localization Lemma 6.12. We reproduce a large part of the proof of Lemma 3.2 in [AEGSS]. However, for the reasons stated in the beginning of Section 6.6, we have to provide an alternative proof of Lemma A.6 in [AEGSS] (Lemma B.4 below) which is the key to the control of the trace-norm.

B.1 Estimates in norm of $\mathscr{B}(\mathscr{H})$

In this section we prove two estimates, uniform in $a \ge 1$ in the norm of $\mathscr{B}(\mathscr{H})$.

Lemma B.1 *Under Hypotheses (H1), (H2), (H3) and (H4) the following estimates hold for all $f \in C_0^\infty(\mathbb{R})$, all $0 < \gamma \le 1$ and all $\varphi \in C^\infty(\mathbb{R})$ such that $\varphi' \in C_0^\infty(\mathbb{R})$.*

(i)

$$\sup_{a \ge 1}\|[f(H), \varphi(\pm A - a)](\gamma(\pm A - a) + \mathrm{i})^m\| < \infty.$$

(ii)

$$\sup_{a,\alpha \ge 1}\langle\alpha\rangle^2\|F((\pm A - a) < -\alpha)[f(H), \varphi(\pm A - a)](\gamma(\pm A - a) + \mathrm{i})^m\| < \infty.$$

Proof. Without loss of generality we may suppose that for $R \equiv \sup\{|x| \,|\, x \in \mathrm{supp}\,\varphi'\} > 0$ we have $\varphi(x) = 0$ if $x < -R$ and $\varphi(x) = L \ge 0$ if $x > R$. We set $A' \equiv \sigma A - a$, with $\sigma \in \{\pm\}$ and we consider

$$\|F(A' \in \mathscr{A})[f(H), \varphi(A')](\gamma A' + \mathrm{i})^m\|.$$

We must show that, uniformly in $a \geq 1$ when $\alpha \to +\infty$, this expression is $O(1)$ if $\mathscr{A} = \mathbb{R}$ and $O(\alpha^{-2})$ if $\mathscr{A} =]-\infty, -\alpha[$ or, equivalently, if $\mathscr{A} =]-\infty, -R\alpha[$. We finally remark that Hypothesis (H4) implies, via Theorem 5.2, that $H \in C^{m+2}_{\text{loc}}(A)$ and thus that $f(H) \in \mathscr{B}^{m+2}_A(\mathscr{H})$.

(i) By invoking Theorem 4.8 we obtain the expansion

$$[f(H), \varphi(A')] = \sum_{j=1}^{m} \frac{(-\mathrm{i}\sigma)^j}{j!} \mathrm{ad}^j_A(f(H))\varphi^{(j)}(A') + R_m, \tag{167}$$

where the remainder is given by the formula

$$R_m = -\frac{(\mathrm{i}\sigma)^{m+1}}{2\pi\mathrm{i}} \int \bar{\partial}\tilde{\varphi}(z)(A'-z)^{-1}\mathrm{ad}^{m+1}_A(f(H))(A'-z)^{-m-1}\,\mathrm{d}z \wedge \mathrm{d}\bar{z},$$

$\tilde{\varphi}$ being the almost-analytic extension of φ of order $m+1$ given by (4) (with $n = m+1$). We easily show, starting from the formula (4), that there exist constants c_1 and c_2 such that $\mathrm{supp}\,\bar{\partial}\tilde{\varphi} \subset \{z = x + \mathrm{i}y \,|\, \langle x\rangle \leq c_1 + c_2|y|\}$. Taking into account the fact that $0 < \gamma \leq 1$ we get that

$$\|(A'-z)^{-m}(\gamma A' + \mathrm{i})^m\| \leq \sup_{a' \in \mathbb{R}} \left|\frac{a' + \mathrm{i}}{a' - z}\right|^m \leq c_3(1 + |\mathrm{Im} z|^{-m}),$$

for all $z \in \mathrm{supp}\,\bar{\partial}\tilde{\varphi}$. With the help of the inequality (5) we obtain the estimate

$$\begin{aligned}\|R_m(A' + \mathrm{i})^m\| &\leq c_4 \int |\bar{\partial}\tilde{\varphi}(x + \mathrm{i}y)|(|y|^{-2} + |y|^{-m-2})\,\mathrm{d}x\mathrm{d}y \\ &\leq c_5 \sum_{j=0}^{m+3} \int \langle x\rangle^{j-2}|\varphi^{(j)}(x)|\,\mathrm{d}x < \infty.\end{aligned}$$

Since, for $j \geq 1$,

$$\|\varphi^{(j)}(A')(\gamma A' + \mathrm{i})^m\| \leq \sup_{x \in \mathbb{R}} |\varphi^{(j)}(x)| \sup_{x \in \mathrm{supp}\,\varphi'} |x + \mathrm{i}|^m < \infty$$

the expansion (167) allows us to conclude that

$$\sup_{a \geq 1} \|[f(H), \varphi(A')](\gamma A' + \mathrm{i})^m\| < \infty.$$

(ii) We set $A_\alpha \equiv -\alpha^{-1}(\sigma A - a) - 2$. We easily verify that $F(A' < -3\alpha) = F(A' < -3\alpha)h(A_\alpha)$ for all $\alpha \geq 1$ and that $h(A_\alpha)\varphi(A') = 0$ for all $\alpha \geq R$. We obtain

$$\begin{aligned}\|F(A' < -3\alpha)[f(H), \varphi(A')](\gamma A' + \mathrm{i})^m\| &\leq \|h(A_\alpha)[f(H), \varphi(A')](\gamma A' + \mathrm{i})^m\| \\ &\leq \|h(A_\alpha)f(H)\varphi(A')(\gamma A' + \mathrm{i})^m\| \\ &\leq \|[f(H), h(A_\alpha)]\varphi(A')(\gamma A' + \mathrm{i})^m\|,\end{aligned}$$

for all $\alpha \geq R$. By applying the expansion (167) to $[f(H), h(A_\alpha)]$, we have

$$[f(H), h(A_\alpha)] = \sum_{j=1}^{m+1} \frac{(\mathrm{i}\sigma\alpha^{-1})^j}{j!} \mathrm{ad}_A^j(f(H)) h^{(j)}(A_\alpha) + R_{m+1}, \tag{168}$$

where the remainder is given by the formula

$$R_{m+1} = -\frac{(-\mathrm{i}\sigma\alpha^{-1})^{m+2}}{2\pi\mathrm{i}} \int \bar{\partial}\tilde{h}(z)(A_\alpha - z)^{-1} \mathrm{ad}_A^{m+2}(f(H))(A_\alpha - z)^{-m-2}\, \mathrm{d}z \wedge \mathrm{d}\bar{z},$$

where $\tilde{h}$ is an almost-analytic extension of order $m+2$. The estimate

$$\|(A_\alpha - z)^{-m}(\gamma A' + \mathrm{i})^m\| \leq \sup_{a' \in \mathbb{R}} \left| \frac{\alpha a' + \mathrm{i}}{a' + 2 + z} \right|^m \leq c_6 \alpha^m (1 + |\mathrm{Im} z|^{-m}),$$

allows us to obtain, as before,

$$\begin{aligned} \|R_{m+1}(\gamma A' + \mathrm{i})^m\| &\leq c_7\, \alpha^{-2} \int |\bar{\partial}\tilde{h}(x + \mathrm{i}y)|(|y|^{-3} + |y|^{-m-3})\, \mathrm{d}x\mathrm{d}y \\ &\leq c_8 \alpha^{-2} \sum_{j=0}^{m+4} \int \langle x \rangle^{j-3} |h^{(j)}(x)|\, \mathrm{d}x \leq c_9 \alpha^{-2}. \end{aligned}$$

Since $h^{(j)}(A_\alpha)\varphi(A') = 0$ for $\alpha \geq R$ and $j \geq 1$, we may conclude that

$$\|F(A' < -3\alpha)[f(H), \varphi(A')](\gamma A' + \mathrm{i})^m\| \leq c_9 \alpha^{-2}.$$

$\square$

We finish this section with a simple lemma.

Lemma B.2 *Under Hypotheses (H1), (H2), (H3), and (H4) we have*

$$\sup_{a \geq 1, \sigma \in \{\pm\}} \|[f(H), 1_k] h_\sigma^{(a)}(A)(\gamma(\sigma A - a) + \mathrm{i})^m\| < \infty,$$

for all $k \in \{0, \ldots, M\}$, $f \in C_0^\infty(\mathbb{R})$ *and* $0 < \gamma \leq 1$.

Proof. An elementary analysis shows that

$$\sup_{x \in \mathbb{R}, \sigma \in \{\pm\}} \left| \left(\frac{\gamma(\sigma x - a) + \mathrm{i}}{x + \mathrm{i}} \right)^m h_\sigma^{(a)}(x) \right| \leq \mu(a)^m \equiv \left(\sup_{x \geq a-1} \frac{1 + (x-a)^2}{1 + x^2} \right)^{m/2},$$

and that $\mu(a) \leq 2$ provided $a \geq 0$. The functional calculus allows us to write

$$\sup_{a \geq 1, \sigma \in \{\pm\}} \|[f(H), 1_k] h_\sigma^{(a)}(A)(\gamma(\sigma A - a) + \mathrm{i})^m\| \leq 2^m \|[f(H), 1_k](A + \mathrm{i})^m\|,$$

and to reduce the proof to the assertion $[f(H),1_k](A+\mathrm{i})^m \in \mathscr{B}(\mathscr{H})$. Since $\widetilde{H}_k \in \mathscr{B}^m_{\widetilde{A}_k}(\widetilde{\mathscr{H}}^1_k, \widetilde{\mathscr{H}}_k)$ by Hypothesis (H4) (ii), Theorem 5.2 implies that $f(H) \in \mathscr{B}^m_{A_j}(\mathscr{H})$ for all $j \in \{0,\dots,M\}$ and we may apply Lemma 4.7 to show that $(A_j+\mathrm{i})^{-m} f(H)(A_j+\mathrm{i})^m \in \mathscr{B}(\mathscr{H})$. Since $1_k A_j = 0$ for $k \neq j$, Lemma 5.1 implies $1_k(A_j+\mathrm{i})^{-m} f(H)(A_j+\mathrm{i})^m = \mathrm{i}^{-m} 1_k f(H)(A_j+\mathrm{i})^m$ from which we conclude that $1_k f(H)(A_j+\mathrm{i})^m$ is bounded. This leads to the result that

$$
\begin{aligned}
[f(H),1_k](A+\mathrm{i})^m &= \sum_{j=0}^{M} \left(1_j f(H) 1_k (A_k+\mathrm{i})^m - 1_k f(H) 1_j (A_j+\mathrm{i})^m\right) \\
&= \sum_{\substack{j=0\\ j\neq k}}^{M} \left(1_j f(H) 1_k (A_k+\mathrm{i})^m - 1_k f(H) 1_j (A_j+\mathrm{i})^m\right),
\end{aligned}
$$

is bounded. □

B.2 The spectral multiplicity of H

We now state a slightly unexpected corollary of Theorem 6.16.

Proposition B.3 *Hypotheses (H1)–(H5) imply that the spectral multiplicity of the Hamiltonian H is locally finite. More precisely, if*

$$
U : \mathscr{H}_{\mathrm{ac}} \to \int^{\oplus} \mathfrak{h}(\varepsilon)\,\mathrm{d}\varepsilon, \tag{169}
$$

denotes the spectral representation associated with the absolutely continuous part of H, then

$$
\int_{\Delta} \dim \mathfrak{h}(\varepsilon)\,\mathrm{d}\varepsilon < \infty,
$$

for all compact $\Delta \subset \mathbb{R} \setminus \Sigma_H$.

Proof. Let $\Delta \subset \mathbb{R}\setminus\Sigma_H$. We consider the charge $Q \equiv I$ and the corresponding current

$$
\widetilde{\Psi}^{\#(a+)}_g \equiv \sum_{k=1}^{M} \widetilde{\Psi}^{\#(a+)}_{g,k} = \sum_{k=1}^{M} g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k), h_+^{(a)}(\widetilde{A}_k) M_k^* M_k h_+^{(a)}(\widetilde{A}_k)] g(\widetilde{H}_k),
$$

where $g \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$, $g=1$ on Δ and $f \in C_0^\infty(\mathbb{R})$. By expanding the commutator we obtain

$$
\begin{aligned}
\widetilde{\Psi}^{\#(a+)}_{g,k} &= g(\widetilde{H}_k)\mathrm{i}[f(\widetilde{H}_k), h_+^{(a)}(\widetilde{A}_k)]\widetilde{\chi}_k^2 h_+^{(a)}(\widetilde{A}_k) g(\widetilde{H}_k) \\
&+ g(\widetilde{H}_k) h_+^{(a)}(\widetilde{A}_k)\mathrm{i}[f(\widetilde{H}_k), \widetilde{\chi}_k^2] h_+^{(a)}(\widetilde{A}_k) g(\widetilde{H}_k) \\
&+ g(\widetilde{H}_k) h_+^{(a)}(\widetilde{A}_k)\widetilde{\chi}_k^2 \mathrm{i}[f(\widetilde{H}_k), h_+^{(a)}(\widetilde{A}_k)] g(\widetilde{H}_k),
\end{aligned}
$$

and it follows from Lemma 6.2 that the second term of the right hand side of this identity is trace-class. The two remaining terms have a similar structure. Writing

$$
[f(\widetilde{H}_k), h_+^{(a)}(\widetilde{A}_k)] g(\widetilde{H}_k) = \left([f(\widetilde{H}_k), h_+^{(a)}(\widetilde{A}_k)](\widetilde{A}_k+\mathrm{i})^m\right)\left((\widetilde{A}_k+\mathrm{i})^{-m} g(\widetilde{H}_k)\right),
$$

Hypothesis (H4) shows that the second factor of the right hand side is trace-class. We easily show, by following the proof of of Lemma B.1 (i), that the first factor is bounded. The current $\widetilde{\Psi}_{g,k}^{\#(a+)}$ is thus trace-class and we may apply Theorem 6.16. The diagonal of its integral kernel is given by

$$\psi_{g,k}(\varepsilon,\varepsilon) = \frac{1}{2\pi} g(\varepsilon)^2 p_k^+(\varepsilon),$$

and it follows from Theorem 6.17 (iii) that

$$\frac{1}{2\pi}\int_\Delta \mathrm{tr}_{\mathfrak{h}_k(\varepsilon)}(p_k^+(\varepsilon))\,\mathrm{d}\varepsilon \le \frac{1}{2\pi}\int g(\varepsilon)^2 \mathrm{tr}_{\mathfrak{h}_k(\varepsilon)}(p_k^+(\varepsilon))\,\mathrm{d}\varepsilon \le \|\widetilde{\Psi}_{g,k}^{\#(a+)}\|_1 < \infty.$$

Since the asymptotic projection P_k^+ commutes with H it admits, in the decomposition (169) the representation

$$(UP_k^+ u)(\varepsilon) = \pi_k^+(\varepsilon)(Uu)(\varepsilon).$$

Moreover, Lemma 6.18 allows us to show that for almost all ε the operators $p_k^+(\varepsilon)$ and $\pi_k^+(\varepsilon)$ are orthogonal projections. Furthermore the intertwining relation $f(H)\Omega_k^+ = \Omega_k^+ f(\widetilde{H}_k)$ implies

$$(U\Omega_k^+ u)(\varepsilon) = \omega_k^+(\varepsilon)(U_k u)(\varepsilon).$$

The relations $\Omega_k^+\Omega_k^{+*} = P_k^+$, $\Omega_k^{+*}\Omega_k^+ = \widetilde{P}_k^+$ and Lemma 6.18 allow us to conclude that

$$\pi_k^+(\varepsilon) = \omega_k^+(\varepsilon)\omega_k^{+*}(\varepsilon), \qquad p_k^+(\varepsilon) = \omega_k^{+*}(\varepsilon)\omega_k^+(\varepsilon),$$

for almost all ε. In particular, we have

$$\mathrm{tr}_{\mathfrak{h}_k(\varepsilon)}(p_k^+(\varepsilon)) = \mathrm{tr}_{\mathfrak{h}(\varepsilon)}(\pi_k^+(\varepsilon)),$$

for almost all ε. It follows from the fact that $\sum_{k=1}^M P_k^+ = P_{\mathrm{ac}}(H)$ that

$$\int_\Delta \mathrm{tr}_{\mathfrak{h}(\varepsilon)}(I)\,\mathrm{d}\varepsilon = \sum_{k=1}^M \int_\Delta \mathrm{tr}_{\mathfrak{h}(\varepsilon)}(\pi_k^+(\varepsilon))\,\mathrm{d}\varepsilon \le 2\pi \sum_{k=1}^M \|\widetilde{\Psi}_{g,k}^{\#(a+)}\|_1 < \infty,$$

which, given the fact that $\dim \mathfrak{h}(\varepsilon) = \mathrm{tr}_{\mathfrak{h}(\varepsilon)}(I)$, concludes the proof. □

B.3 Trace-norm estimates

The following lemma is the key to control the trace-norm in the proof of Lemma 6.12.

Lemma B.4 *Under Hypotheses (H1)–(H5),*

$$\sup_{a\in\mathbb{R},\sigma\in\{\pm\}} \|(\gamma(\sigma A - a)+\mathrm{i})^{-m} g(H)\|_1 < \infty,$$

for all $g \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$ *and* $\gamma > 0$ *sufficiently small.*

Proof. We set $T \equiv (\gamma(\sigma A - a) + \mathrm{i})^{-1}$ and, without loss of generality, we suppose that

$$\sup_{x\in\mathbb{R}} |g(x)| \le 1.$$

We begin by showing that $T^m g(H)$ is trace-class. We have

$$T^m g(H) = \sum_{k=0}^{M} (\gamma(\sigma A_k - a) + \mathrm{i})^{-m} 1_k g(H),$$

where the $k = 0$ term is bounded uniformly by Hypothesis (H4) (iii),

$$\|(\gamma(\sigma A_0 - a) + \mathrm{i})^{-m} 1_0 g(H)\|_1 = \|(-\gamma a + \mathrm{i})^{-m} 1_0 g(H)\|_1 \le \|1_0 g(H)\|_1.$$

For $k \in \{1,\dots,M\}$ Hypothesis (H1) (v) and the identity (107) imply that $(1_k - \chi_k^2)1_k^{(2)} = (1_k^{(2)} - \chi_k^2)1_k^{(2)} = 0$. Hypothesis (H1) (iii) allows us to conclude that $(1_k - \chi_k^2) = (1_k - \chi_k^2)1_0^{(2)}$. It follows from this identity and from (134) that

$$\begin{aligned}
(\gamma(\sigma A_k - a) + \mathrm{i})^{-m} 1_k g(H) &= M_k(\gamma(\sigma \widetilde{A}_k - a) + \mathrm{i})^{-m} M_k^* g(H) + (-\gamma a + i)^{-m}(1_k - \chi_k^2) g(H) \\
&= M_k(\gamma(\sigma \widetilde{A}_k - a) + \mathrm{i})^{-m} g(\widetilde{H}_k) M_k^* \\
&\quad + M_k(\gamma(\sigma \widetilde{A}_k - a) + \mathrm{i})^{-m} (M_k^* g(H) - g(\widetilde{H}_k) M_k^*) \\
&\quad + (-\gamma a + i)^{-m}(1_k - \chi_k^2) 1_0^{(2)} g(H).
\end{aligned}$$

The first term on the right hand side of this identity is trace-class by Hypothesis (H4) (i). Lemma 6.1 shows that the second term is trace-class. Finally, the last term is trace-class by Hypothesis (H4) (iii).

We now show that $T^m g(H)$ is uniformly bounded in $\mathscr{L}^1(\mathscr{H})$. Let $f \in C_0^\infty(\mathbb{R}\setminus\Sigma_H)$ such that $0 \le f \le 1$ and $fg = g$. We begin with the identity

$$T^m g(H) = f(H) T^m g(H) + [T^m, f(H)] g(H). \tag{170}$$

By invoking Lemma 4.7 to expand the commutator of the second term of the right hand side of this identity we obtain

$$[T^m, f(H)] = \sum_{j=1}^{m} \binom{m}{j} (\mathrm{i}\gamma\sigma)^j T^j \mathrm{ad}_A^j(f(H)) T^m \equiv B T^m.$$

Hypothesis (H4) (ii) and Theorem 5.2 allow us to estimate

$$\|B\| \le \sum_{j=1}^{m} \binom{m}{j} \gamma^j \|\mathrm{ad}_A^j(f(H))\| \le C\gamma,$$

for a constant C and γ small enough. We may thus conclude from identity (170)

$$\|T^m g(H)\|_1 \le \|f(H) T^m g(H)\|_1 + C\gamma \|T^m g(H)\|_1,$$

and conclude that for $\gamma < (2C)^{-1}$ we have

$$\|T^m g(H)\|_1 \le 2\|f(H)T^m g(H)\|_1.$$

Since $g = fg$ and $|g| \le 1$ we may also write

$$\|T^m g(H)\|_1 \le 2\|f(H)T^m f(H)\|_1 \le 2\|f(H)|T|^m f(H)\|_1 = 2\,\mathrm{tr}(f(H)|T|^m f(H)).$$

We consider now the spectral representation (169). Since the spectrum of H is purely absolutely continuous on $\operatorname{supp} f$ we have

$$f(H)|T|^m f(H) = P_{\mathrm{ac}}(H)f(H)|T|^m f(H)P_{\mathrm{ac}}(H),$$

and Theorem 6.17 allows us to conclude that this operator has an integral kernel $c(\varepsilon,\varepsilon') \in \mathscr{L}^1(\mathfrak{h}(\varepsilon'),\mathfrak{h}(\varepsilon))$ such that

$$\mathrm{tr}(f(H)|T|^m f(H)) = \int_{\operatorname{supp} f} \mathrm{tr}(c(\varepsilon,\varepsilon))\,\mathrm{d}\varepsilon.$$

Lemma 6.19 implies

$$\begin{aligned}\int (u(\varepsilon), c(\varepsilon,\varepsilon)u(\varepsilon))_{\mathfrak{h}(\varepsilon)}\,\mathrm{d}\varepsilon &= \lim_{\eta\downarrow 0}\int_{-\infty}^{\infty} \mathrm{e}^{-\eta|t|}(u, \mathrm{e}^{-\mathrm{i}tH}f(H)|T|^m f(H)\mathrm{e}^{\mathrm{i}tH}u)\,\mathrm{d}t\\ &= \lim_{\eta\downarrow 0}\int_{-\infty}^{\infty} \mathrm{e}^{-\eta|t|}\||T|^{m/2}f(H)\mathrm{e}^{\mathrm{i}tH}u\|^2\,\mathrm{d}t. \qquad (171)\end{aligned}$$

We shall estimate this last integral. We note that for all $\alpha \ge 0$ we have

$$\||T|^{m/2}F(\gamma|\sigma A - a| > \alpha)\| \le \langle\alpha\rangle^{-m/2},$$

and thus

$$\begin{aligned}&\||T|^{m/2}f(H)\mathrm{e}^{-\mathrm{i}\sigma tH}f(H)|T|^{m/2}\|\\ &\quad\le \|F(\gamma|\sigma A - a| \le \alpha)\mathrm{e}^{-\mathrm{i}\sigma tH}f(H)^2F(\gamma|\sigma A - a| \le \alpha)\| + 3\langle\alpha\rangle^{-m/2}\\ &\quad\le \|F(\gamma(\sigma A - a) \le \alpha)\mathrm{e}^{-\mathrm{i}\sigma tH}f(H)^2F(\gamma(\sigma A - a) \ge -\alpha)\| + 3\langle\alpha\rangle^{-m/2}.\end{aligned}$$

Setting $\alpha = \gamma\vartheta t/2 \ge 0$, Hypothesis (H4) (i) and Theorem 5.2 allow us to apply Proposition 4.27 to obtain

$$\|F(\gamma(\sigma A - a) \le \gamma\vartheta t/2)\mathrm{e}^{-\mathrm{i}\sigma tH}f(H)^2F(\gamma(\sigma A - a) \ge -\gamma\vartheta t/2)\| \le c\langle\vartheta t\rangle^{-s},$$

for constants c and $s > 1$, uniformly in a. We thus have

$$\||T|^{m/2}f(H)\mathrm{e}^{-\mathrm{i}\sigma tH}f(H)|T|^{m/2}\| \le c_1\left(\langle t\rangle^{-s} + \langle t\rangle^{-m/2}\right),$$

for $t \ge 0$. This inequality extends to all $t \in \mathbb{R}$ by taking the adjoint. Taking into account the fact that

$$|T|^{m/2}f(H)(H-z)^{-1}f(H)|T|^{m/2} = \pm\mathrm{i}\int_0^{\infty} |T|^{m/2}f(H)\mathrm{e}^{\mp\mathrm{i}t(H-z)}f(H)|T|^{m/2}\,\mathrm{d}t,$$

we get

$$\sup_{z\in\mathbb{C}\setminus\mathbb{R}} \||T|^{m/2} f(H)(H-z)^{-1} f(H)|T|^{m/2}\| \leq c_2,$$

for all $a \geq 1$. By invoking Theorem XIII.25 of [RS4] and its corollary we obtain

$$\int_{-\infty}^{\infty} \||T|^{m/2} f(H) \mathrm{e}^{\mathrm{i}tH} u\|^2 \,\mathrm{d}t \leq c_3 \|u\|^2,$$

with $c_3 = 2c_2$. Relation (171) thus allows us to write

$$0 \leq \int (u(\varepsilon), c(\varepsilon,\varepsilon) u(\varepsilon))_{\mathfrak{h}(\varepsilon)} \,\mathrm{d}\varepsilon \leq \int (u(\varepsilon), c_3 u(\varepsilon))_{\mathfrak{h}(\varepsilon)} \,\mathrm{d}\varepsilon,$$

from which we get $\mathrm{ess}-\mathrm{supp}_{\varepsilon\in\mathbb{R}} \|c(\varepsilon,\varepsilon)\| \leq c_3$ and

$$\mathrm{tr}_{\mathfrak{h}(\varepsilon)}(c(\varepsilon,\varepsilon)) \leq c_3 \mathrm{tr}_{\mathfrak{h}(\varepsilon)}(I),$$

for almost all ε. Consequently

$$\begin{aligned}
\|T^m g(H)\|_1 &\leq 2\mathrm{tr}(f(H)|T|^m f(H)) \\
&= 2\int_{\mathrm{supp}\, f} \mathrm{tr}(c(\varepsilon,\varepsilon)) \,\mathrm{d}\varepsilon \\
&\leq 2c_3 \int_{\mathrm{supp}\, f} \mathrm{tr}_{\mathfrak{h}(\varepsilon)}(I) \,\mathrm{d}\varepsilon \\
&\leq c_4 < \infty,
\end{aligned}$$

by an application of Proposition B.3. □

B.4 Proof of Lemma 6.12

Since $h_\sigma^{(a)}(0) = 0$ for $a \geq 1$, Lemma 5.1 implies

$$h_\sigma^{(a)}(A) = \sum_{j=0}^{M} 1_j h_\sigma^{(a)}(A_j) 1_j,$$

and thus $h_\sigma^{(a)}(A_k) = 1_k h_\sigma^{(a)}(A) = h_\sigma^{(a)}(A) 1_k$ which allows us to write, with $A' \equiv \sigma A - a$, $0 < \gamma < 1$ and $\mathscr{A} \subset \mathbb{R}$

$$\begin{aligned}
\|F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A_k)] g(H)\|_1 &= \|F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A) 1_k] g(H)\|_1 \\
&\leq \|F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A) 1_k](\gamma A' + \mathrm{i})^m\| \, \|(\gamma A' + \mathrm{i})^{-m} g(H)\|_1.
\end{aligned}$$

If $\gamma > 0$ is sufficiently small, the second factor of the right hand side of this inequality is uniformly bounded for $a \in \mathbb{R}$ by Lemma B.4. We must thus control the first factor and show that it is uniformly bounded if $\mathscr{A} = \mathbb{R}$ and that it decreases as $\langle \alpha \rangle^{-s}$ uniformly in a if $\mathscr{A} =]-\infty, -\alpha[$.

From $h_\sigma^{(a)} = h_\sigma^{(a-2)} h_\sigma^{(a)}$ we obtain

$$h_\sigma^{(a)}(A)1_k = h_\sigma^{(a-2)}(A) h_\sigma^{(a)}(A)1_k = h_\sigma^{(a-2)}(A)1_k h_\sigma^{(a)}(A),$$

and thus

$$\begin{aligned}[f(H), 1_k h_\sigma^{(a)}(A_k)] &= [f(H), h_\sigma^{(a-2)}(A)]1_k h_\sigma^{(a)}(A) + h_\sigma^{(a-2)}(A)1_k[f(H), h_\sigma^{(a)}(A)] \\ &\quad + h_\sigma^{(a-2)}(A)[f(H), 1_k] h_\sigma^{(a)}(A),\end{aligned}$$

then

$$\begin{aligned}&F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A)1_k](\gamma A' + \mathrm{i})^m \\ &\quad = F(A' \in \mathscr{A})[f(H), h_\sigma^{(a-2)}(A)](\gamma A' + \mathrm{i})^m h_\sigma^{(a)}(A)1_k \\ &\quad + 1_k h_\sigma^{(a-2)}(A) F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A)](\gamma A' + \mathrm{i})^m \\ &\quad + h_\sigma^{(a-2)}(A) F(A' \in \mathscr{A})[f(H), 1_k] h_\sigma^{(a)}(A)(\gamma A' + \mathrm{i})^m.\end{aligned}$$

In the corresponding estimate

$$\begin{aligned}&\|F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A_k)](\gamma A' + \mathrm{i})^m\| \\ &\quad \le \|F(A' \in \mathscr{A})[f(H), h_\sigma^{(a-2)}(A)](\gamma A' + \mathrm{i})^m\| \\ &\quad + \|F(A' \in \mathscr{A})[f(H), h_\sigma^{(a)}(A)](\gamma A' + \mathrm{i})^m\| \\ &\quad + \|h_\sigma^{(a-2)}(A) F(A' \in \mathscr{A})\| \, \|[f(H), 1_k] h_\sigma^{(a)}(A)(\gamma A' + \mathrm{i})^m\|,\end{aligned} \tag{172}$$

the second factor of the last term of the right hand side is uniformly bounded for $a \ge 1$ by Lemma B.2. The first factor is uniformly bounded for $a \in \mathbb{R}$ and vanishes when $\mathscr{A} \cap [a-3, \infty[$ is empty. In particular, for all $s > 0$ there exists a constant C_s such that

$$\|h_\sigma^{(a-2)}(A) F(\sigma A < a - \alpha)\| \, \|[f(H), 1_k] h_\sigma^{(a)}(A)(\gamma(\sigma A - a) + \mathrm{i})^m\| \le C_s \langle \alpha \rangle^{-s},$$

for all $a, \alpha \ge 1$. The two first terms of the right hand side of (172) are both of the form

$$\|F(A' \in \mathscr{A})[f(H), \varphi(A')](\gamma A' + \mathrm{i})^m\|,$$

where $\varphi' \in C_0^\infty(]-3, 1[)$ and $0 \le \varphi \le 1$. Applying Lemma B.1 completes the proof. □

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